Project No. 15-8843

Development of Accident Tolerant Fuel Options For Near Term Applications

Integrated Research Project

Mujid Kazimi

Massachusetts Institute of Technology

Collaborators

Texas A&M University

University of Florida

University of Wisconsin at Madison

Suibel Schuppner, Federal POC

Jon Carmack, Technical POC

NEUP Nuclear Energy University Programs

U.S. Department of Energy

Development of Accident Tolerant Fuel Options
For Near Term Applications

Final Report

Oct 2015 through Dec 2018 (3.25 years)

Mujid Kazimi (Principal Investigator)*
Koroush Shirvan (Executive Director)
Thomas McKrell (Collaborator)*
**Deceased*
Department of Nuclear Science and Engineering
Massachusetts Institute of Technology

Kumar Sridharan (Collaborator)
Michael Corradini (Collaborator)
Department of Engineering Physics
University of Wisconsin at Madison

Lin Shao (Collaborator)
Department of Nuclear Engineering
Texas A&M University

Michael Tonks (Collaborator)
Department of Material Science and Engineering
University of Florida

Jason Hales (National Lab Collaborator)
Fuel Modeling and Simulation
Idaho National Laboratory

Jeffrey Reed (Industry Collaborator)
Fuel Commercial & Customer Center
Framatome

Wenfeng Liu (Industry Collaborator)
Structural Integrity Associates, Inc.

Contents

Acknowledgments

The following integrated research project (IRP) was originally led by Professor Mujid Kazimi of Nuclear Science and Engineering (NSE) Department at Massachusetts Institute of Technology (MIT). Without Prof. Kazimi's leadership and experience in this area the formation of such unique team would not have been possible. Professor Kazimi's sudden passing in July 2015 provided major blow to the NSE department and the IRP. Many thanks for Professor Jacopo Buongiorno for providing leadership when needed to take over Prof. Kazimi role and act as a senior advisor to the project. The efforts of Dr. Thomas McKrell who was in charge of the experimental activities of the IRP at MIT require a special acknowledgment before his unfortunate passing in 2017. In addition following individuals are acknowledged:

At MIT, Professor R. Ballinger, Research Scientists: Dr. B. Philips and L. Snead, Students: Y. Che, Y. Deng, A. Gurgen, M. Sevecek, A. Seshadri, M. Wagih, J. Petrik, W. McGhee and Post-Docs: Y. Sukjai, W. Li, X. Wu

At University of Wisconsin-Madison, co-PI Dr. Kumar Sridharan and Professor Michael Corradini and their students: T. Dabney, G. Johnson, B. Maier; Research Scientists: J. Wang, H. Yeom

At Texas A&M University, co-PI Professor Lin Shao and students/postdocs: J. Gigax , M. Kennas, E. Ryabikovskaya, A. French, H. Kim

At University of Florida, co-PI Professor Michael Tonks and student: F. Hilty

At Structural Integrity, co-PI Dr. Wenfeng Lui and Dr. Joe Rashid and Dr. Nathan Capps

At Framatome, co-PI Jeff Reed and Chris Lewis, Brian Mays, and Kiran Nimishakavi

At Idaho National Laboratory: Co-PI Jason Hales and Giovanni Pastore, and Ben Spencer

Outside participants who contributed to our monthly project calls and yearly workshops include Michael Todosow and Lap-Yan Cheng from Brookhaven National Laboratory and Frank Goldner from DOE office of nuclear energy.

Funding for this work has been provided by DOE IRP contract # DE-NE0008416

Preface

The final report serves as the summary of the following listed 11 milestones totaling *602 page*s delivered previously to DOE during the IRP by the IRP members:

1. Completion of fabrication of all Coated Cladding Samples [38 pages]

2. Completion of Ion Irradiation of ATF Concepts [43 pages]

3. Experimental evaluation of corrosion and mechanical Performance of Coated Cladding Samples under normal operating conditions [51 pages]

4. Experimental evaluation of corrosion and mechanical Performance of Coated Cladding Samples under severe accident conditions [52 pages]

5. CHF and Quench Testing of Promising Cladding Candidates [69 pages]

6. Neutronics Model Development and Analysis [13 pages]

7. Thermal-Hydraulic Model Development and Safety Analysis [104 pages]

8. Fuel performance modeling under normal operation [74 pages]

9. Fuel performance modeling under transients/severe accident conditions [115 pages]

10. Integration of Tools for Time to Failure Analysis [24 pages]

11. Economic Evaluation of ATF Concepts for Near Term [19 pages]

The findings in these 11 milestones have been further documented in 12 published (see section 4) and 7 submitted journal publications. Annual workshops were also held to disseminate the detail findings of the study among the project collaborators as well as outside attendees including representation from all major fuel vendors in the US, Electric Power Research Institute and Nuclear Regulatory Commission. The final report also includes recommended future work reflected through discussion with the project participants and a white paper detailing gaps in coated clad technology (Appendix A). Overall, the IRP highlights a successful execution of a public-private partnership among multiple university, national lab and industry collaborators.

Disclaimer: The following final report summary may only represent the views of the project executive director with supporting contributions from the project collaborators.

Koroush Shirvan
Executive Director
Assistant Professor
Dept. of NSE, MIT

1. Background

1.1 IRP FOA and Workscope

In this section, the basis for the proposal followed by description of the work scope and methodologies are discussed. Following the Fukushima disaster in 2011, US congress mandated the department of energy to start a R&D program on accident tolerant fuel (ATF) concepts for the existing light water reactor fleet. By 2015, the start date of this IRP, several ATF concepts were being pursued by various entities. In general, the ATF concepts were divided into two categories: near term and long term. The near term concepts included: Coated Zircaloy clad, fuels with additives and dopants and FeCrAl/steel based claddings. The long term concepts included: SiC composite cladding, high density fuels (U_3Si_2, UN) and TRISO type fuel forms (e.g. FCM). It is of particular importance for any DOE funded effort to give background information and original Funding Opportunity Announcement (FOA) goals in its final report to evaluate whether the FOA goals and the proposed work were actually addressed.

The FOA for this IRP sought for modeling and simulation capability to predict various ATF performances during normal operation, design basis accident and severe accident conditions. Particularly, the FOA was concern with the state of the core performance during a severe accident. It was postulated that if an ATF retains its structural integrity, the performance of non-fuel structures in the core needs to be addressed. The IRP team focused the proposal on Pressurized Water Reactor (PWR) performance for near term ATF concepts: Coated cladding, Fuel with additives and dopants to accelerate adoption of such concepts and address the unanswered questions regarding their performance. The project also gave limited focus on another near term concept, FeCrAl cladding, by restricting its scope to time-to-failure prediction since substantial effort supported by other programs including ORNL ATF program, GEH ATF program and NEAMS High Impact Problem[1] were already made or underway during the IRP tenure.

Despite two previous IRPs funded in 2012 with focus on experimental study of metallic and ceramic Zircaloy coated claddings[2], this IRP still included a coating program. This was a testament to the project leadership's belief that the coated clad concept will be the primarily initial pathway

[1] https://inldigitallibrary.inl.gov/sites/sti/sti/Sort_3383.pdf

[2] https://neup.inl.gov/SitePages/FY12%20IRP%20Awards.aspx

for near term industrialization of ATF technology due to presence of enrichment penalty and licensing hurdles of the alternative clad concepts. In doing so, the IRP was positioned to provide key findings on coated Zircaloy as a uniquely funded external program to DOE's industrial ATF campaign. Currently, in 2019, the coated clad concept is being pursued by all three vendors for licensed application and Lead Test Rods and Lead Test Assemblies (LTRs/LTAs) have already been inserted or planned to be inserted in the existing fleet.

At the start of the IRP project, based on the meeting with the projects technical and federal point of contacts, it was also agreed upon if the contractual obligations are met, then the scope of the simulation work will be extended to Boiling Water Reactors as included in Section 2.10.

1.2 Experimental Component

The primary goal of the experimental work under this IRP was to provide critical data for the coated cladding concept for time-of-failure analysis and to support the ATF campaign experimental objectives. In this IRP, total of <$1 million was allocated for experimental work. Since the leadership of the IRP were nuclear engineering design experts, rather than material scientists, the approach was inherently different than the previous mentioned IRPs on coated clad. Traditionally, experimental programs of new concepts are focused on typical coupon size testing and developing a reliant fabrication process. In a university environment this typically takes multiple years and not a very fruitful endeavor within the typical 3 year time frame of DOE funded projects. In this IRP, the experimental work was focused on testing unique specimens in prototypic LWR normal and accident conditions in order to specifically provide the ATF concepts failure modes to inform the simulation component of the IRP. Such methodology taken in this IRP, as will be highlighted and supported by the key findings in the next section is believed to be an asset and basis for future acceleration of nuclear fuel R&D both in terms of time and cost.

Two parallel coating programs were pursued for the IRP, one led by UW and one led by MIT. For both efforts, the base material for the coatings was Zircaloy-4, in form of solid rods, hollow tubes and plates as shown in Fig. 1. The Zirc-4 specimens were obtained from FRAMATOME (Formerly known as AREVA at the start of the IRP). Then MIT fabricated over 80 samples into geometries that are compatible with various testing facilities at MIT to be coated by UW (shown in Figure 1) and external vendors.

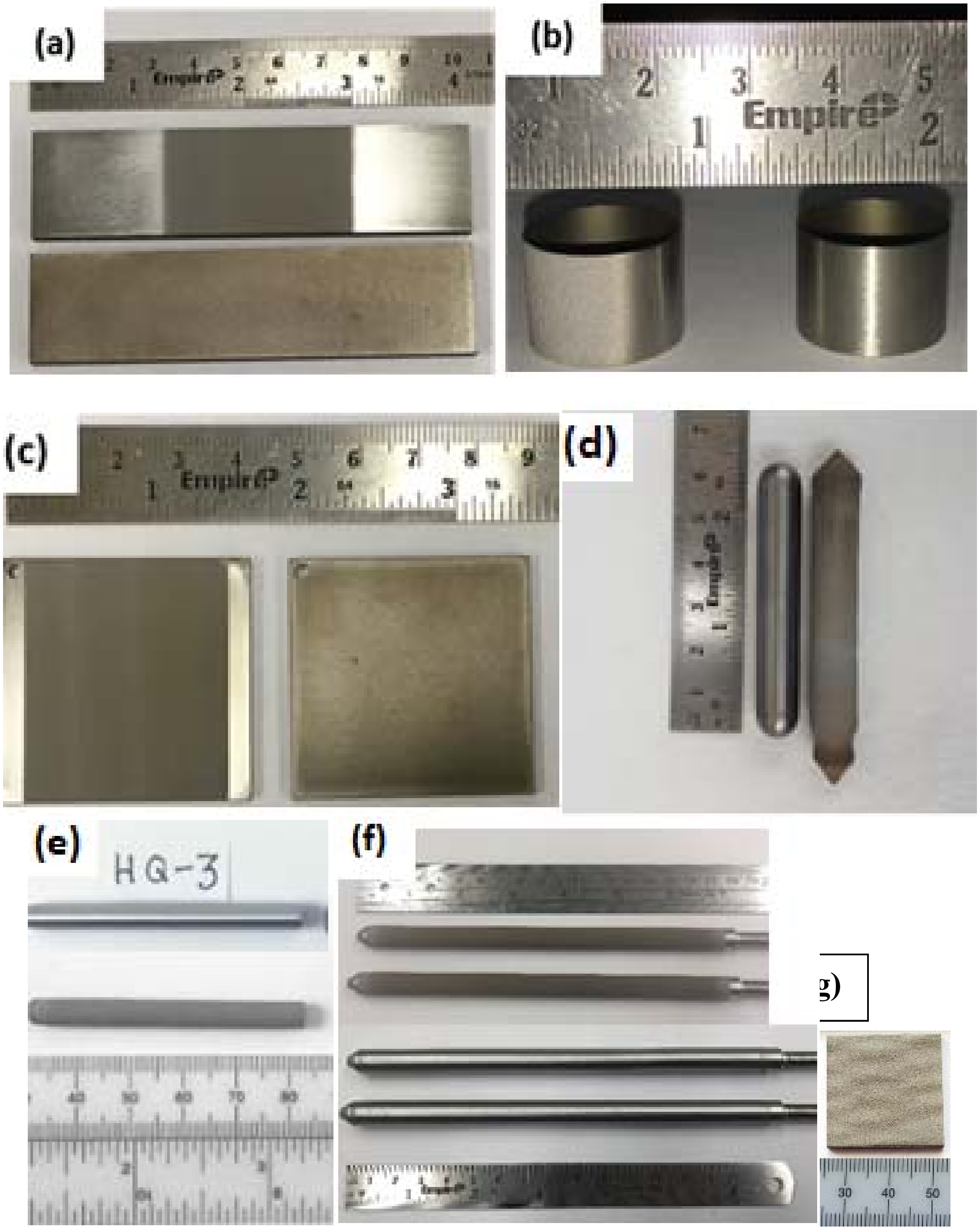


Figure 1: (a) 14x 4-point bend specimen for fatigue cycling tests at BWR and PWR pressure, temperature and water chemistry (b) 9x CRUD tube samples for CRUD affinity tests at PWR pressure, temperature, water chemistry with added corrosion products under heat flux (c) 16x Steam oxidation coupons for 500 ºC steam oxidation to investigate steam oxidation resistance and nodular corrosion behavior (d) 6x High temperature steam samples to investigate protectiveness of the coating at 1200 to 1500 ºC steam (e) 6x Hydraulic quench specimen for performance high temperature quench (600 to 1500ºC) experiments (f) 10x Pressure Tube rodlets for stress corrosion and cracking testing at BWR and PWR prototypic conditions and high temperature oxidation behavior beyond melting (1200-1500ºC) (g) 3x Ion Irradiation coupons to understand the coating-substrate interface performance under irradiation.

University of Wisconsin (UW) with their fabrication capability focused on cold-spray (CS) Mo/FeCrAl cladding concept as providing the Cr coating was not possible due to presence of non-disclosure agreements by the time the project was awarded. UW obtained FeCrAl and Molybdenum powders for the coating effort. UW also performed polishing of most of the specimens to obtain smooth surface finish. In some cases, UW also applied a FeCrAl overcoat on the Moly samples, since Moly is high corrosive under high temperature water and steam. But Mo serves as a diffusion barrier to slow down the Fe and Zr low melt eutectic formation. The coatings were also mechanically characterized, showing high hardness and more wear resistance compared to Zirc-4. For testing, the coated samples were shipped to MIT. While the UW coated material concept is not currently being pursued by any vendor, it still required a significant effort to apply the coating material using the cold-spray process for the complex geometries. The aim of this effort was to leverage lessons learned for chromium coated Zircaloy concept.

At MIT, in order to follow the original proposal and remain industry relevant, discretionary funds were spent to fabricate cold-spray Chromium coated samples. Army Labs and Plasma Pros provided CS Cr coating for the IRP.

The overall testing campaign was divided into four general categories:

1. Ion irradiation of coated specimens: Systematic studies by Texas A&M University (TAMU) have been performed to understand interface reactions between coating layers and Zircaloy-4 substrate, formation of interface compounds, and radiation responses of each interface zone.
2. Thermal-Hydraulic Performance: The replacement of Zirconium in a nuclear reactor with other materials will change the coolant-surface heat transfer. Prior to the integrated research project (IRP) start date and the start date of this milestone, there has been numerous studies on quantification of Critical Heat Flux of accident tolerant fuel concepts under pool boiling inclusive of the ones considered in this study. In Oct 2018, DOE started 4 different NEUPs on this topic alone. Thus, the IRP focus was narrowed to quench heat transfer of various ATF concepts (Cr, FeCrAl, Mo) by MIT.
3. Corrosion Performance: It was important to confirm the ability of the coatings to suppress corrosion relative to Zircaloy-4 as well as its response to high temperature which was less known at the time of the award. High temperature and high pressure water autoclave tests with and without hydrogen along with low temperature and high temperature steam tests

were performed. In addition the IRP did some of the early work on >1200 ºC test where eutectic formation between Cr and Zirc-4 concept was observed.

4. Mechanical Performance: Creep testing was performed to demonstrate how the coating will change Zirc-4 creep behavior. Burst testing was performed at low and high temperatures to measure the burst pressure and burst size. In addition, fatigue testing was performed to understand the durability and impact of coating on substrate performance.

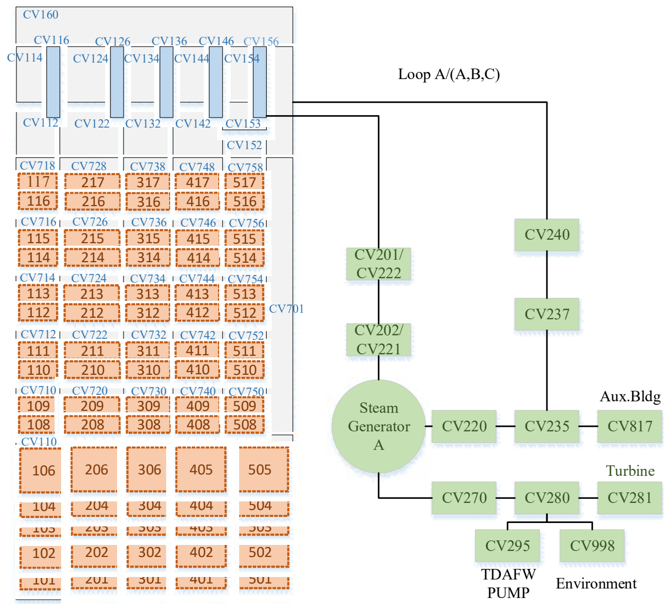
1.3 Modeling and Simulation Component

As mentioned, the original intent of the FOA for the IRP was to focus on modeling and simulation (M&S) to predict time-to-failure. Similar to the experimental component, strong effort was made to avoid duplication of previous and planned M&S work. The contribution of the modeling work was rationalized in terms of coping time calculations, fuel performance simulations and economic impact analysis.

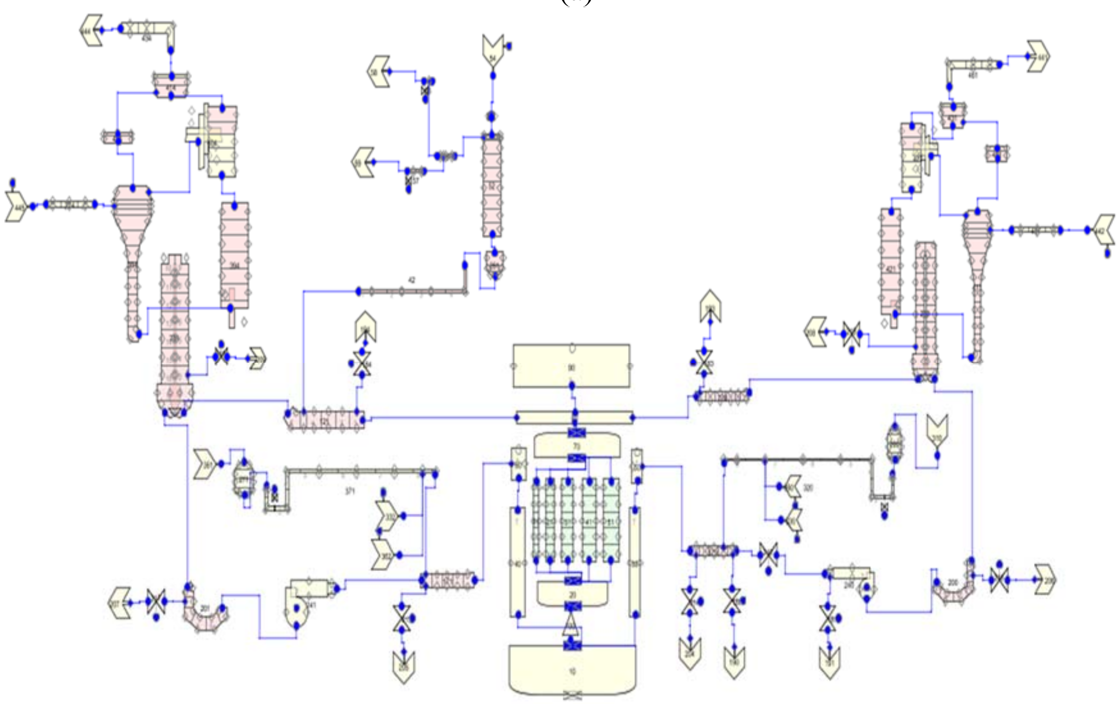
For the coping time calculations, a new approach of using a best estimate system code to predict time-to-failure was developed. This was motivated by the fact that severe accident type codes such as MAAP and MELCOR, typically lacked the fine detail that best estimate system codes are able to provide in the initial phase of the severe accident progression which is critical for time-to-failure analysis vs. the actual severe accident consequences. Two different system level codes were utilized in this work: Nuclear Regulatory Commission (NRC) severe accident code MELCOR at UW and NRC's best estimate system code TRACE at MIT. Both codes were utilized to estimate ATF coping time for a reference 3-loop Pressurized Water Reactor (PWR) shown Figure 2.

UW used the MELCOR Surry model obtained from Sandia National laboratories (SNL).[3] UW also obtained an ATF version of MELCOR from INL that is able to model FeCrAl cladding.[4] MIT created a reference 3-Loop PWR based specification given by BNL PWR model developed as part of DOE Fuel Cycle Technologies R&D Program. [5] MIT then developed and implemented FeCrAl and Cr material properties and severe accident models into the TRACE source code.

[3] Bixler, N.E., Brewer, J.D., Brock, T., et al., 2008, Volume II, NUREG/CR, SAND2008P
[4] Merrill, B.J., Bragg-Sitton, S.M., Humrickhouse, P.W., 2015, INL/EXT-13-30206, Rev.2
[5] Cheng, L-Y., et al., BNL-107113-2015-CP, (2014)



(a)



(b)

Fig. 2: (a) MELCOR Surry Plant Model – SOARCA – SNL nodalization and (b) 3-Loop PWR model nodalization in TRACE.

The secondary goal of this effort was to verify TRACE best estimate prediction at conditions close to fuel meltdown with MELCOR's more mature severe accident models. Thus, for the first time, the MELCOR/TRACE benchmark was also performed for Zircaloy and ATF cladding FeCrAl for a reference PWR benchmark specification at temperatures considered as beyond design basis accident (BDBAs) .i.e. severe accidents. Later in the project, detailed BWR modeling was also performed.

For fuel performance simulations, there was no published work on how chromium coating would behave on Zirc-4 cladding as proposed by ATF stakeholders and continues to-date to be an original contribution of the IRP. The fuel performance of Zirc/Mo/FecrAl fuel system as proposed by EPRI was also assessed and is discussed in the next section. The M&S work covered fuel performance under normal, power ramps and design basis accident conditions such as Loss of Coolant Accident (LOCA) and Rod Ejection Accidents (REA). For REA full core reactor physics simulations were performed to demonstrate the negligible impact of coated or FeCrAl cladding on REA outcome.

For doped fuel, currently pursued under the ATF campaign by both FRAMATOME and Westinghouse, the existing engineering scale fuel performance validation and simulation works were limited in open literature. Also, doped fuel postulated performance under a LOCA had not been explored in detail previously. MIT led such M&S work by utilizing the BISON fuel performance tool in collaboration with INL and FRAMATOME. Additionally, University of Florida led work on UO_2 fuel with BeO/SiC additives. This work aimed to demonstrate the value of meso-scale modeling and serve as a model for lower scale modeling to inform engineering scale phenomena and experimental programs to accelerate R&D.

No attempts were made for fuel performance simulation for beyond design basis accident due to limitation of BISON code capability and the marginal predicted gain in coping time by adopting near term cladding concepts.

The replacement of Zirconium or introduction of other materials in a nuclear reactor will impact the cost of nuclear fuel from enrichment requirement point-of-view. Prior to this IRP start date, there has been numerous studies on quantification of economic impact of near term ATF options on fuel cost. Thus, reactor physics calculations in this work focused on additional cost of enrichment by applying the coating on guide tubes and non-fuel components which was not investigated previously. Beyond the fuel cost, the economic impact of introduction of ATFs on safety, risk-informed programs and other areas of nuclear power plant operation and maintenance were also estimated.

2. Summary of Key Findings

2.1 Mo/FeCrAl Coating Testing Outcome

Overall, it appeared that FeCrAl coated cladding samples exhibited corrosion and oxidation behavior similar to commercially available bulk FeCrAl alloys in normal operating conditions. Slight deviation from this behavior came from the microstructure of the coatings, which were found to contain a higher density of pores after testing. Characterization of these coatings before testing was not performed extensively, but as-deposited cold spray coatings produced by UW have not been found to contain any cracks. These cracks (see Figure 3) likely originated from faults in the as-deposited coating such as pores, and proliferated due to the extreme nature of the testing. Additionally, thermal expansion coefficient mismatch between Zircaloy-4 and FeCrAl (Zr-4 thermal expansion is about half that of FeCrAl) and aggressive thermal cycling likely contributed to this behavior. Further optimization of the cold spray process to produce dense FeCrAl coatings devoid of pores would likely increase the oxidation resistance and delay porosity formation in severe conditions.

Both alloy composition and surface preparation were found to have some impact on the corrosion behavior of FeCrAl coated cladding candidates. While higher alloy additions of Cr and Al should increase the corrosion resistance of FeCrAl alloys, these polished coatings were found to either have formed an extremely thin oxide layer or no oxide layer at all after extended testing, which may have been due to spallation. Meanwhile, the lower alloy FeCrAl coatings with higher Fe content were found to produce a continuous oxide layer on the surface of the coatings. The low-alloy FeCrAl coatings also sealed cracks with a Fe-rich oxide more, demonstrating the self-healing property of FeCrAl alloys. No significant oxide formation in cracks and pores was observed in the high-alloy FeCrAl coatings. Interestingly, FeCrAl coatings left in the as-sprayed condition and thus having considerable surface roughness formed a very thick multi-layered oxide on the surface with various compositions, though the reason for this observation is not known.

The addition of the Mo diffusion barrier coating was shown to have positive results. On its own, the Mo coating was not protective as an accident tolerant coating due to its propensity for oxidation. At normal operating conditions, Mo oxidizes forming stable MoO_2; however, as temperatures exceed normal operating temperatures, Mo readily oxidizes to form volatile MoO_3, leading to evaporation of the coating and reducing its life as a coating. The Mo coating as an interlayer, however, showed some positive results. It became clear from high temperature tests that

Mo oxidation and volatilization was possible if oxygen diffused through cracks in the outer FeCrAl coating towards the Mo interlayer. Even so, much of that oxygen remained trapped in the Mo interlayer, thus preventing oxidation of the Zr-alloy substrate.

Additionally, Fe and Cr diffusion into the substrate was entirely prevented by this Mo diffusion barrier – this was the intended primary function of the layer given the high diffusion kinetics of Fe into Zr and the low eutectic melting point between the two elements. No severe inter-diffusion of Fe into the substrate occurred, which is the main degradation mechanism of a FeCrAl coating on a Zr-alloy substrate. Since the Mo diffusion barrier prevented Fe, Cr, and O diffusion from reaching the substrate, the Mo interlayer effectively provided an extra layer of protection for the underlying Zr-alloy substrate. Optimization of the cold spray process for the outer FeCrAl coating would further help make FeCrAl/Mo a successful coated-cladding concept in terms of oxidation and corrosion resistance. Further characterization and analysis of the mechanical performance of the coatings in normal and severe conditions will need to be assessed in the future.

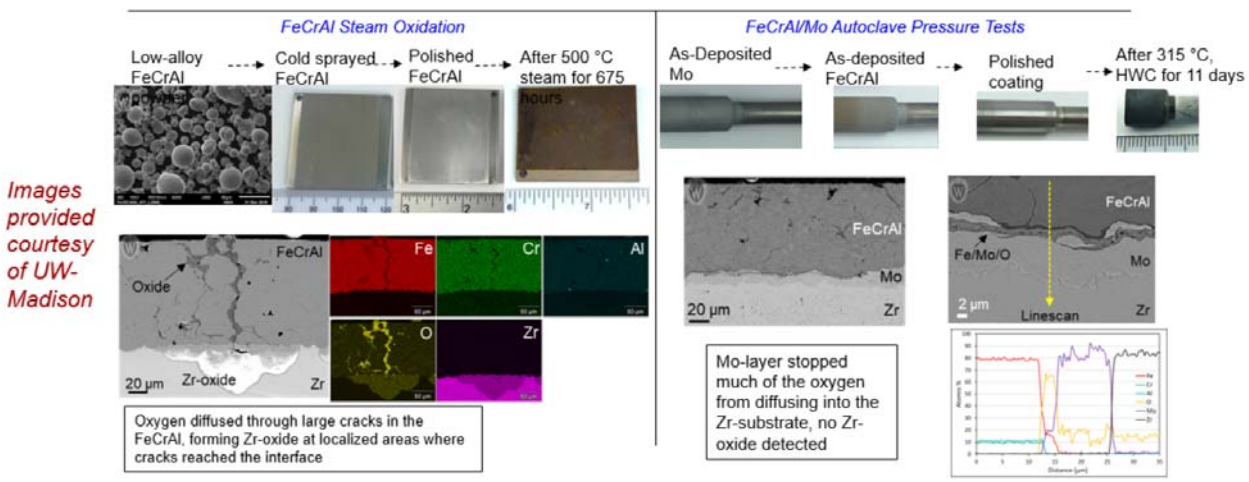
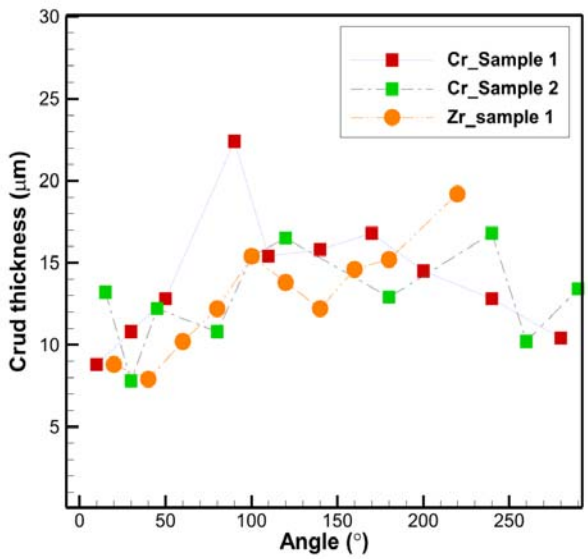


Figure 3. Selected post-test examinations by UW on the FeCrAl/Mo coating.

2.2 Cr Coating Testing Outcome

The Cr coating proved to be a promising concept as supported by continual industrial development. The coating process, quality and findings are documented in existing papers in literature as part of this IRP.[6,7,8,9] While newer findings that have not been published are also summarized in this section. The 500ºC steam oxidation tests showed substantially reduced oxidation measured on the basis of weight gain and later confirmed by microscopy relative to Zirc-4. The coating roughness also contributed to its weight gain as its weight gain was higher than the tested pure chrome specimen. Almost no difference was observed in terms of CRUD deposition for two independent four week long tests in a flowing CRUD loop. The azimuthal CRUD distribution along the specimen (see Fig. 1b) for one of the tests is shown in Figure 4 (left). Multiple creep testing showed stability of the coating under both compression and tension. The creep strain between the coated clad and uncoated was found to be similar based on 1200 hours of testing at 360ºC and 400ºC at ~120 MPa hoop stress. High temperature burst (800ºC) showed much less ballooning and longer burst time for the Cr coating as shown in Fig 4, in-line with existing results by FRAMATOME in literature. None of the post-characterized mechanical or thermal tests resulted in coating spallation.



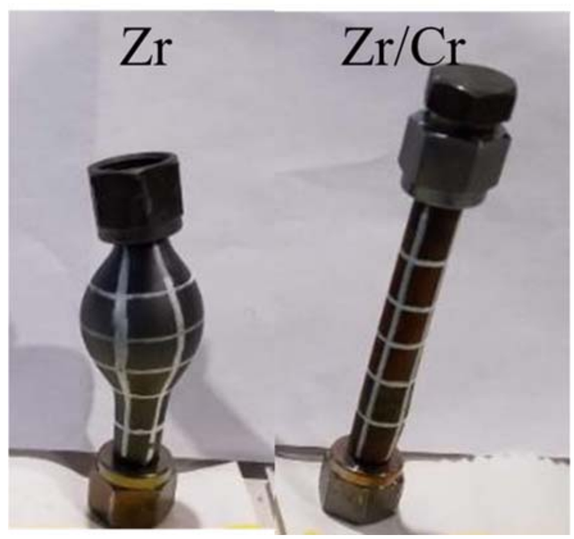


Figure 4. Azimuthal CRUD thickness after 4 week of flow testing in PWR-type water chemistry on CRUD specimens (See Figure 1) (left) and post-test burst visualization after exposure to 800ºC and 4 MPa internal pressure for 450 sec and 2000 sec for Zirc-4 and Cr coated Zirc (Zr/Cr), respectively [To be published in Topfuel 2019].

[6] Seshadri A., Shirvan K., *"Quenching Heat Transfer Analysis of Accident Tolerant Coated Fuel Cladding,"* Nuclear Engineering and Design, Vol. 338 pp. 5-15, 2018.
[7] Sevecek M., et al., *"Development of Cr Cold-Sprayed Fuel Cladding with Enhanced Accident Tolerance,"* Nuclear Engineering and Technology Journal, Vol 50, pp. 229-236, 2018.
[8] Shahin M., Petrik J., Seshadri A., Philips B., Shirvan K., *"Experimental Investigation of Cold-Spary Chromium Cladding,"* Topfuel, Prague Oct 2018.
[9] Sevecek M., Krijci J., Shahin M., Petrik J., Ballinger G., Shirvan K., *"Fatigue Behavior of Cold-Spray Coated Accident Tolerant Cladding,"* Topfuel, Prague Oct 2018.

Relative to Zirc-4, more brittle fracture and crack propagation were observed in our cold-spray Cr coating post thermal and mechanical testing. These defects and failure modes are currently attributed to the cold-spray process parameters and how the underlying Zircaloy microstructure is impacted during the deposition process. CS in general generates a non-uniform interface as shown in Figure 3, creating stress concentrators and can reduce fatigue lifetime depending on the CS process parameters as shown experimentally in our IRP (See Figure 5 and Reference 9). It is believed that through the optimization of the process as well as utilization of modern Zircaloy material such adverse behavior could be avoided. When it comes to other low temperature techniques, such as PVD technique used by FRAMATOME, the underlying Zircaloy surface remains smooth and unperturbed. However, as result, it is likely that not as strong of a bond is formed between the two materials. If cracks are formed due to combination of manufacturing defects or mechanical loads, then a localized oxide will be formed in the underlying Zirc-4. This localized oxidation, as visualized by Figure 3 (lower left), can also act as a stress concentrated and increase the brittle fracture, crack propagation and reduce the fatigue lifetime of the cladding. Such highlighted failure mode is critical for the industry and the regulator to address in the near future.

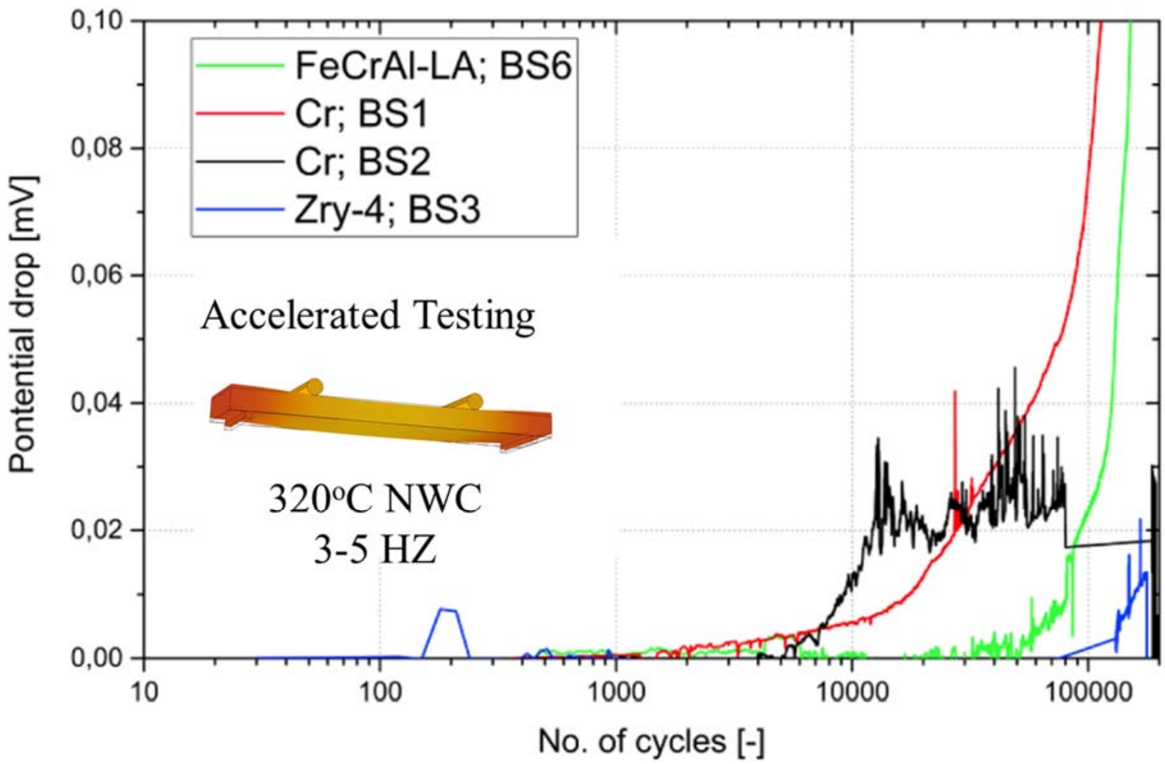


Figure 5. Earlier crack detection for Cr and FeCrAl CS coated Zirc-4 vs. uncoated Zirc-4 [9].

In summary, based on the IRP testing program, four new failure modes for the coated clad, particularly metallic Chromium, have been discovered. The first one is described above and illustrated in Fig. 5 while the other 3 are illustrated in Fig. 6.

1. Clad damage by the coating: The importance of Zircaloy surface microstructure on its corrosion and mechanical performance has been historically demonstrated and led to different processes and Zirconium-based alloys. Similarly the coating process will impact this microstructure depending on the coating process parameters. Also, any cracks in the coating could result in its propagation in the Zircaloy substrate by creating a stress concentrator or localized corrosion/hydrogen pickup sink. Impact of radiation on the coating material could also further contribute to this damage mechanism.
2. Coating/Zirconium High Temperature Interaction: At 1330ºC, Zirconium and Chromium form a eutectic. This will result in formation of a brittle intermetallic compound, loss of ductility and different clad collapse/melt progression for severe accidents. The coating process parameters in terms of presents of pre-existing oxides or impurities will impact the rate of formation of the eutectic and inter-diffusion of Cr in Zirconium. The Cr diffusion may not result in formation of a compound but it may embrittle the cladding.
3. Rod bowing during accidents: Typically rod bowing is a failure mechanism during normal operation and AOOs that would impact the fuel critical heat flux and thermal margins. In case of coated clad, only a nano-meter thick oxide is formed on the cladding, while the Zircaloy metal underneath loses all of its strength at > 800 ºC. Therefore, the fuel is more susceptible to bowing, bending and buckling, especially if the fuel-clad chemical bond is not present.
4. Subsurface oxide driven cracking: Zirconia is a porous material that can rapidly form under high temperature steam evironment. In case of presence of crack or manufacturing defects such as near the end-plug zone, the formation of Zirconia layer under the metallic coated layer can result in propagation of cracks, while the outer surface of the rod continues to be very ductile at high temperature conditions. This failure mode, similar to the 2 and 3 is likely a phenomena that could be observed during severe accidents.

Appendix A provides a more detailed view of how the chromium coated clad will impact current fuel licensing limits.

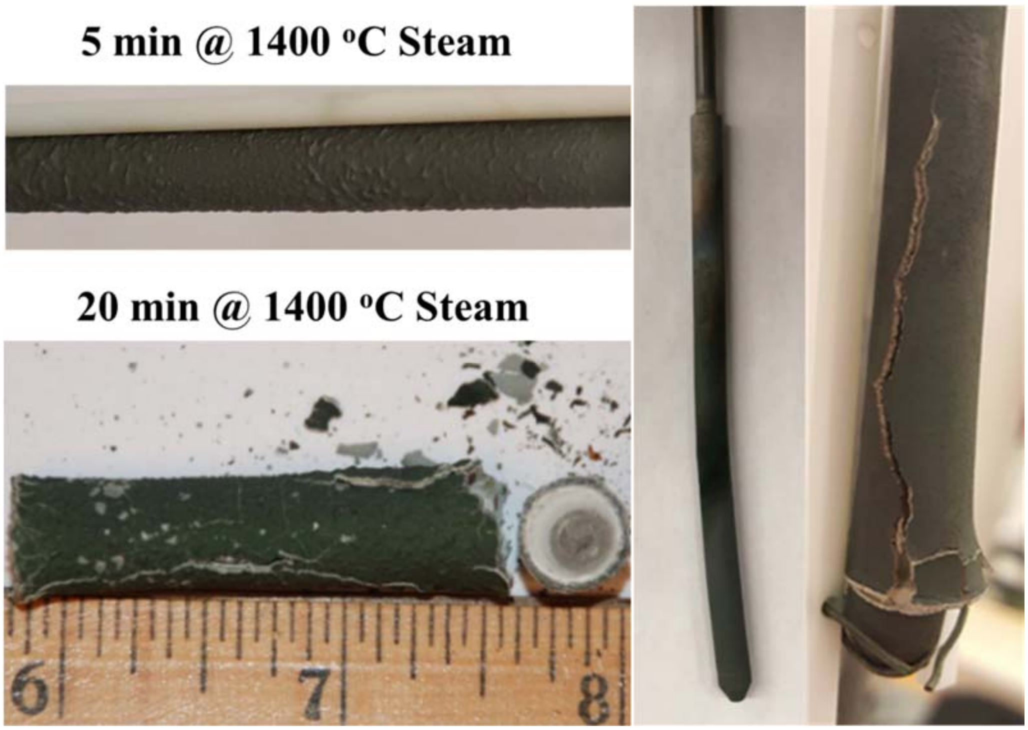


Figure 6. Failure mode 2: Formation of Cr-Zirconium eutectic at >1330ºC (left), Failure mode 3: bending of the Cr coated Zirc (middle), and Failure mode 4: crack initiation at the weld region were coating was not applied continuously and its propagation axially across the rodlet (right).

2.3 Ion Irradiation Testing Outcome

The TAMU work focused on three coating materials: Ti_2AlC (MAX phase), FeCrAl and Cr.

For Ti_2AlC coating, we identify three interface compounds, $ZrAl_2$, ZrAl, and Zr_3Al. Diffusion of Al atoms plays a dominant role in influencing intermetallic phase formation. The diffusion kinetics of Al are estimated by measuring the widths of the intermetallic layers. The activation energy is determined to be ~202 kJ/mol. All three interface phases are amorphized after 3.5 MeV Zr ion irradiation to 100 peak dpa. MAX phase has significant structural distortion. Nanoindentation reveals hardening of Ti_2AlC, Zr_3Al, and the Zircaloy-4 substrate after irradiation.

For FeCrAl coating, a mixed Zr_2Fe/ZrC phase and Zr_3Fe form at the interface. The formation energies of these two phases are found to be 68 kJ/mol and 46 kJ/mol for Zr_2Fe (mixed with ZrC) and Zr_3Fe, respectively. Nanoindentation and micropillar compression tests on site-selected regions of cross sections of polished samples obtain different mechanical responses. The Zircaloy-4 shows the lowest hardness and most ductile deformation under compression, and interfacial

Zr_2Fe and Zr_3Fe layers possess the highest hardness and brittle deformation. 3.5 MeV Zr ion irradiation is performed to reach damage levels of 50, 100 and 150 peak dpa (displacements per atom). No voids are found within the coating layer and the substrate. However, ZrC is easily amorphized at 50 dpa and higher damage levels.

Comparison studies suggest that (1) cold-spray coating technique is suitable to form tightly bonded coating/substrate system. Kinetic energy of injected powders is able to induce athermal atomic mixing which benefits adhesion, as shown by our cantilever bending experiment; (2) interface compound formation follows an Arrhenius relation, hence the width changes under arbitrary annealing conditions can be estimated using diffusion kinetics extracted from the present studies; (3) MAX phase shows poorer radiation tolerance in comparison with FeCrAl. Significant structural distortion is found after 100 dpa irradiation, due to structural collapse in the presence of high density anti-site defect formation; (4) interface compound layers between MAX phase coating and Zircaloy-4 have low radiation tolerance and these layers become amorphized after irradiation; (5) C contamination during cold spray process induce a ultra-thin layer of ZrC which is easily amorphized after ion irradiation.

For chromium coating, no homogenous phase formation was observed after exposing the CS sample to 725 ºC for 6 weeks in vaccum, as supported by Figure 7. It was observed that some inter-diffusion of Cr in Zirc in form of few micron may have occurred. No Cr was found ~5 microns away from the interphase. A separate study on ion-irradiation induced swelling of the pure chrome was also performed. This work was motivated by the complete gap in literature on impact of neutron irradiation on Cr swelling. The ion irradiation was performed with 5.0 MeV Fe^{2+} for cumulative dpa of 50-150 at $1x10^{-3}$ dpa/s. The substrate temperature was kept between 450-650 ºC. The averaged swelling is shown in Figure 8, hinting that Cr-coating swelling may not be negligible as currently assumed in the fuel performance models. Since the Cr coated samples were independently fabricated by MIT, due to budget availability and time, detailed mechanical evaluation of irradiated coated Cr specimen was not performed and is reserved as future work.

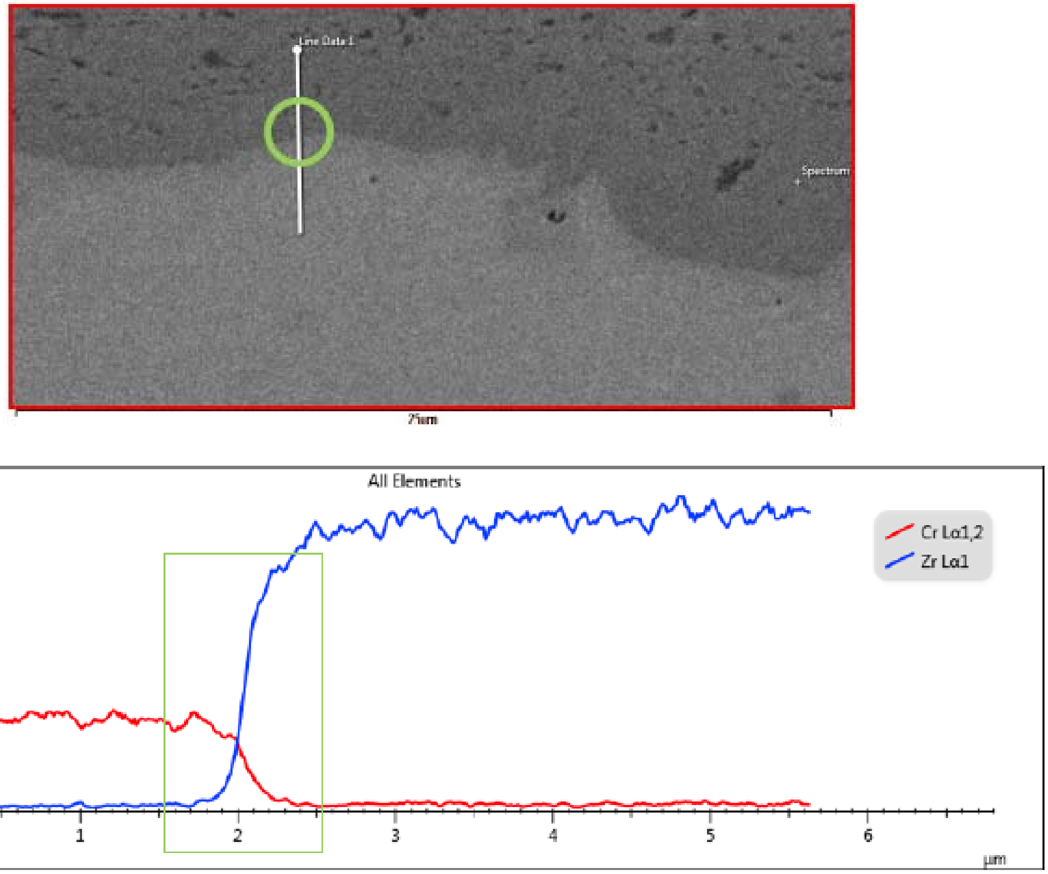


Figure 7. EDS line scan (below) of the interphase region (Top) indicates no clear homogeneous phase has formed.

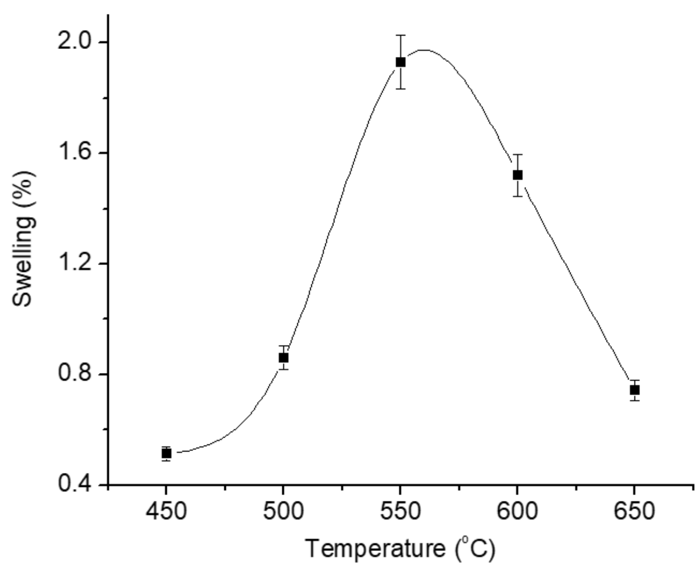


Figure 8. Averaged Chromium swelling (from 200 to 600 nm) as a function of temperatures (all for 50 peak dpa irradiation).

2.4 Quench Heat Transfer Behavior Testing Outcome

In this study, several key insights in quench performance of ATF cladding as well as the fundamental understanding of impact of gamma radiation based on surface chemistry were made for the first time[6,10].

1. Radiation induced surface activation (RISA) from gamma irradiation plays a vital role in understanding the wettability and quench performance of tested surfaces.
2. RISA effect depends on the surface chemistry and material properties
3. Mechanism behind enhancement of surface wettability for gamma irradiation is different than UVO where gamma irradiation has permanent effect in the surface as shown clearly in Fig. 9 due to formation of oxide micropores. This permanent effect is observed at high temperatures (> 300 ºC) as in lower temperature, the contaminants remain intact.
4. Mechanistic model considering the surface chemistry and irradiation effect is needed to properly define the boiling and quench performance of irradiated materials.
5. It was observed that FeCrAl had a better cooling characteristic when compared to Zircaloy-4 both with non-oxidized and oxidized samples (see Figure 10). Chromia had the best cooling performance among all the tested candidates.
6. Detailed surface characterization supported with microscopic and profilometry analysis revealed that porosity and surface roughness had significant impact in improving the cooling in the oxidized samples.
7. The nature of the porosity (micro or nano) had a decisive role in enhancing the capillary wicking (nucleate boiling cooling rate) during the nucleate boiling regime and also the Leidenfrost temperature both in cases of oxidized and non-oxidized samples

These findings are valuable in guiding future DOE funded project to ensure effect of radiation and oxidation is properly taken into account. Also, valuable insights were found through measurement of surface characteristics beyond contact angle. In particular, surface chemistry and porosity, while its quantification is not well-understood, play an important role in heat transfer rate. As for Cr coating, given the worse measured quench cooling rate, a LOCA simulation showed that its impact on the figure-of-merit (peak cladding temperature) is not significant since the exothermic reaction by Zr with high temperature steam is reduced by the Cr coating as shown in Fig. 11.

---

[10] Seshadri A., Philips B., Shirvan K., "*Towards Understanding the Effects of Irradiation on Quenching Heat Transfer,*" Journal of Heat and Mass Transfer, Vol 127 pp. 1087-1095, 2018.

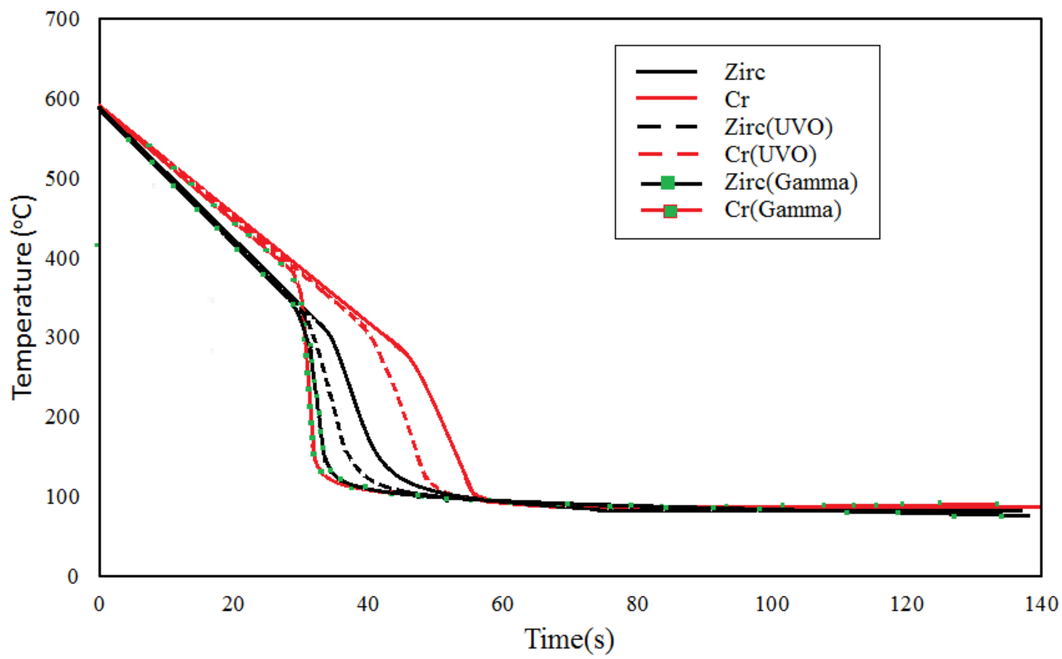


Fig. 9 Quench time history for non-irradiated samples, gamma irradiated samples and UVO treated samples

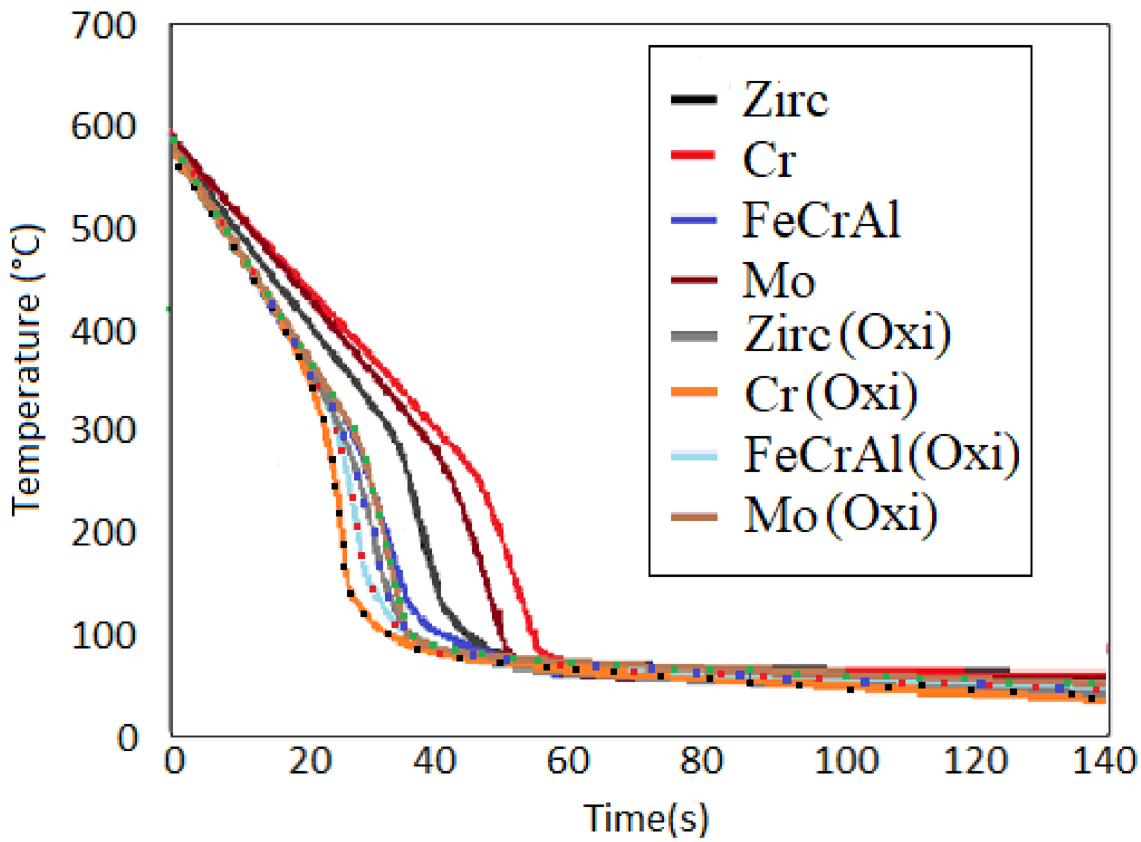


Fig. 10 Temperature history during the Quenching of Oxidized rodlets (Tmax=600 °C)

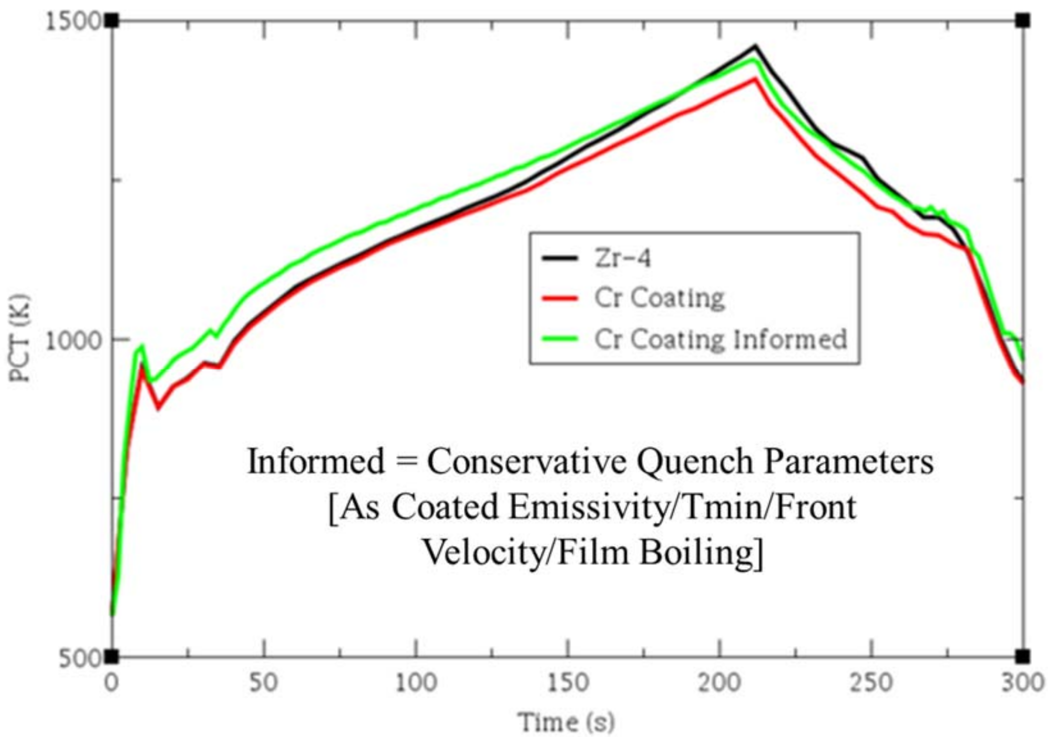


Figure 11. Peak clad temperature (PCT) during a large-break LOCA for a BWR (Note, the simulated LOCA for Zr-4 was setup such that current PCT limit of ~1200ºC is reached in order to clearly demonstrate the impact of worse quench heat transfer of Cr-coating on safety).

2.5 Reactor Physics Simulation

In this study, our utilization of realistic core reload design and use of commercial tools (STUDSVIK) to simulate reactor core Neutronics from full core point-of-view led to different conclusions than previously DOE supported work. Estimation of enrichment decrement due to introduction of ATF cladding on assembly basis overestimates the enrichment decrement vs. full core estimate. It was found that assembly level calculations match the full core calculations if the Kinfinities of the ATF cladding and referenced Zirc-4 cladding are matched at burnup of 25 MWD/kgU. This is much lower than the assumed 40 MWD/kgU in many previous studies.[11] During reactivity insertion accidents (RIA) it was found that for a given inserted reactivity (e.g. $1.25), there was no difference in the predicted maximum deposited fuel enthalpy among the claddings as shown in Figure 12. The choice of a single limiting reactivity worth is consistent with current regulatory demands. The use of state-of-art commercial reactor simulator show that the ATF cladding will result in similar performance and there is no need

[11] I. Younker et al., Progress in Nuclear Energy 88 (2016) 10-18

to change the REA testing procedures. These findings are valuable in guiding future DOE funded project to ensure more rigorous analysis that involves code-to-code comparison is supported.

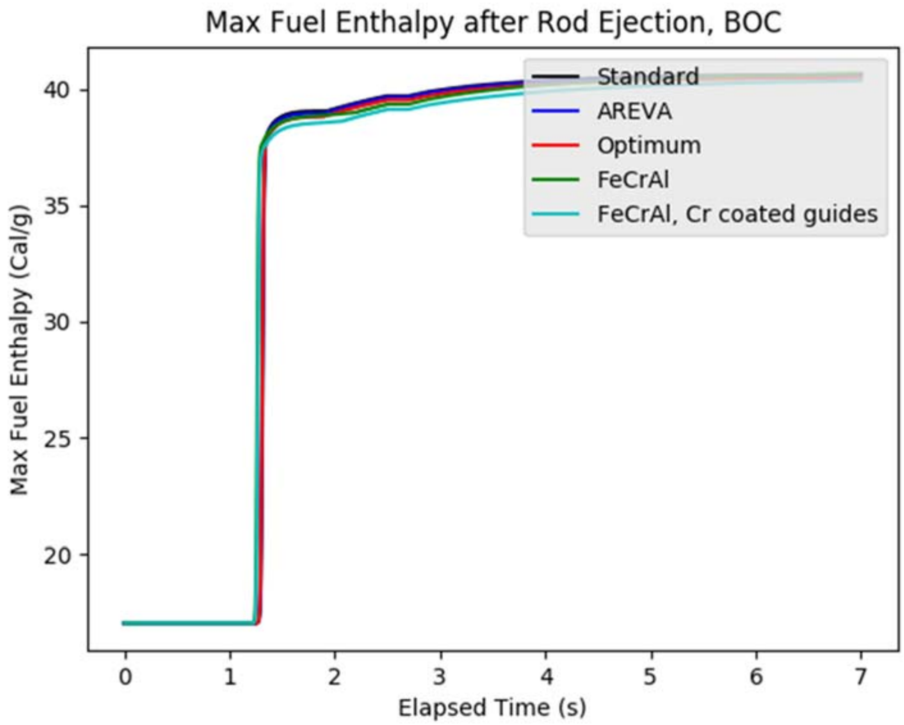


Figure 12. Maximum fuel enthalpy during REA for standard (UO2/Zr), AREVA (Doped UO2/Cr-coated Zirc), Optimum (AREVA + Coating on guide tubes), FeCrAl (UO2/FeCrAl clad and guide tubes) and FeCrAl and Cr coated Guide tubes simulated by Simulate3K code package.

2.6 Thermal-Hydraulic System Modeling and Simulation

The major finding of this work was that introduction of oxidation resistant claddings such as FeCrAl show *notable but modest* gains in coping time under various scenarios including unmitigated large break loss-of-coolant accident and short term and long term station black out for the 3-loop PWR reactor system.[12,13,14] The coping time was also found to be function of the chosen figure of merit (FOM). In our work, the primarily FOMs, were time to onset of significant hydrogen production (~kg) and time to onset of cladding melt for MELCOR and TRACE codes, respectively. It was found that the degree of dependence of the coping time on a particular FOM

[12] Wang J., et al., *"Accident tolerant clad material modeling by MELCOR: benchmark for surry short term station black out,"* Nuclear Engineering and Design, Vol 313 pp. 458-469, 2017.
[13] Gurgen, A., Shirvan, K., *"Estimation of coping time in pressurized water reactors for near term accident tolerant fuel claddings"*, Nuclear Engineering and Design, Vol 337 pp. 38-50, 2018.
[14] J. Wang, H. J. Jo & M. L. Corradini, *"Potential Recovery Actions from a Severe Accident in a PWR: MELCOR Analysis of a Station Blackout Scenario,"* Nuclear Technology, 204:1, 1-14, 2018.

depends on a particular accident scenario. These major findings played an important role in the industry-led ATF program in the US.

Specifically, UW led MELCOR work considered accident tolerant cladding material (e.g., FeCrAl alloy: APMT) and its effect on the accident behavior. In this research, UW used clad oxidation and associated hydrogen generation as the figure of merit, which can determine the time window following Auxiliary Feedwater (AFW) failure before hydrogen generation becomes significant from oxidation of metallic cladding (Zircaloy vs. FeCrAl) during a station blackout sequence. A parametric analysis was carried out using a novel analysis method for a range of assumed AFW failure times and one finds that the time to initial hydrogen generation are increased before clad oxidation and fuel degradation begins while ATF cladding materials are used as shown in Fig. 13. This suggests that ATF cladding materials have the potential of expanding the time window for recovery actions during a LWR severe accident.

In MIT-led TRACE work, the performances of the FeCrAl and Cr-coated ATF claddings under beyond design basis accidents (BDBA) are modeled. Two models are used for high-temperature oxidation of FeCrAl: a model based on the experimental results of this IRP, and a model based on experimental results of ORNL's work. In this IRP, FeCrAl was exposed to fast temperature ramps, and its failure was predicted to occur at 1375ºC vs. ORNL assumed >1500 ºC based on slower temperature ramp oxidation tests. The following BDBAs are simulated for this study: large break loss of coolant accident (LOCA) without safety injection systems, short-term station blackout (SBO) without any mitigation actions from the beginning and long-term SBO with auxiliary feedwater flow for the first 24 hours and the no mitigation actions afterwards. The effect of oxidation of control rods and guide tubes were also considered separately. The peak cladding temperature for the long term SBO is shown in Fig. 14. The results showed that ATF claddings increase the coping time and produce less hydrogen compared to Zircaloy cladding under the considered BDBAs scenarios. When considering the FOM of time to reach clad melt, the gains in coping times was found to be marginal, especially for the coated claddings.

A benchmark comparison with MELCOR and TRACE was also conducted based on a simplified generic PWR model for a short-term station black out. Through the simulation and analysis, we can come to the conclusion that: 1) Calculated thermal hydraulic parameters are quite similar for MELCOR and TRACE, for either Zircaloy or FeCrAl cladding cases up to 1500 K at which a noticeable deviation starts to occur. 2) More importantly, the gain in coping time by FeCrAl cladding ability to significantly decrease the hydrogen generation mass in the initial stages of the core heat up was the same for both MELCOR and TRACE calculations.

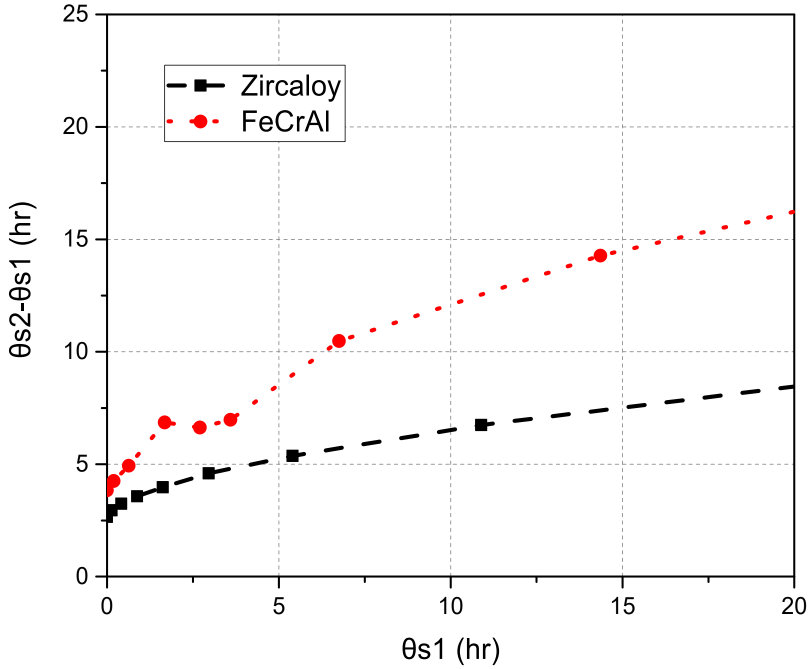


Figure 13. Comparison of the Time Delay between AFW failure (x-axis) and Hydrogen Generation for Zircaloy Clad and ATF FeCrAl Clad Material (y-axis).

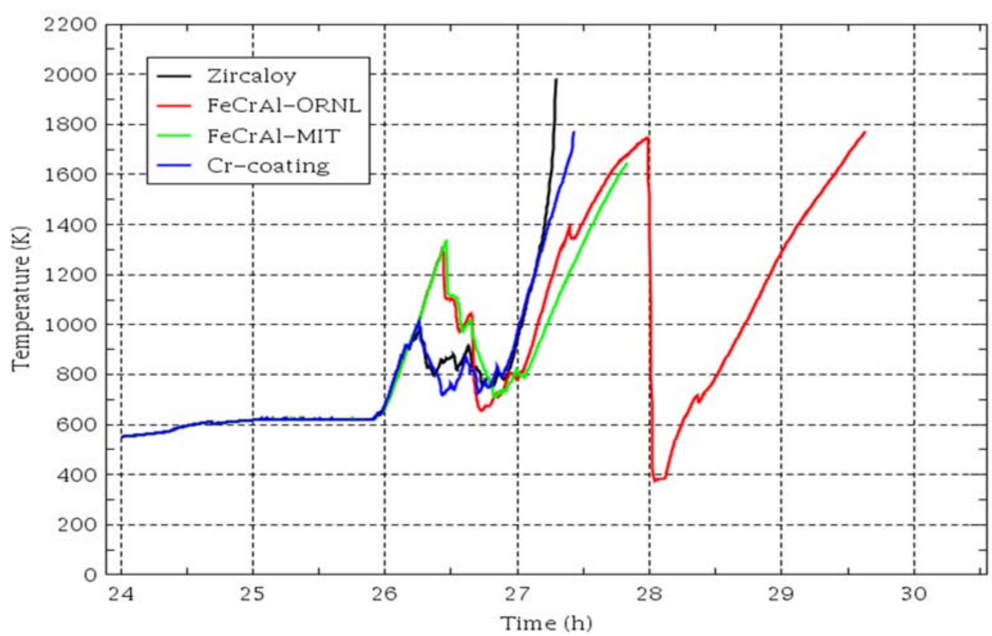


Figure 14: TRACE peak cladding temperature profile for long-term SBO after 24 hours for cladding systems.

2.7 Normal and AOO Fuel Performance Simulations of Near Term ATFs

The fuel performance simulation for normal and AOO were divided into four categories:

1. Zr4-Chromium coated cladding (see Fig. 15) [Led by MIT]
2. Zr4-FeCrAl coated cladding with a molybdenum interlayer (see Fig. 15) [Led by MIT]
3. Chromia Doped Fuel (Large grain pellets) [Led by MIT, FRAMATOME and INL]
4. UO_2 fuel with BeO/SiC additives (See Fig. 16) [Led by University of Florida (UF), formally by Pennsylvania State University (PSU)]

The coated claddings were kept to a 50μm of coating thicknesses, deducted from the base layer thicknesses. The doped and additive content were kept as found in literature for model validation. All four of the ATF concepts were studied, using MOOSE-based multi-physics tools, under steady-state PWR operating conditions.

The major finding is that the chromium coated concepts proved to be the most promising coated cladding concept, while the Zr4-Mo/FeCrAl cladding showed high plastic strains in the molybdenum layer relative to what Mo can handle, making its possibilities of survival questionable. The impact of coating on major fuel performance parameters such as fuel temperature and cladding creep was found to be small under normal operating conditions, simulated with the INL's BISON fuel performance tool. Though, uncertainty still exists as the coating performance is both function of fabrication technology and irradiated material properties that are not readily available at this time. Fig. 17 shows the effective stress and plasticity in each of the coating layers as a function of time.

The feasibility of modeling the chromia doped fuel behavior under normal operation in BISON was confirmed based on Halden data. It was found that the mechanistic fission gas release model in BISON can capture the doped fuel performance when the fuel grain size and diffusion coefficient are modified based on experimental observation. Though, significant uncertainty exists in the BISON fission gas release model parameters as confirmed by a comprehensive sensitivity analysis. Fig. 18 shows the predicted average fission gas release by BISON and its one sigma uncertainty in its prediction vs. the measured steady-state fission gas release. The available validation data from Halden did not include power ramps, the key benefit of doped fuel and the FRAMATOME power ramp database is proprietary. Therefore, a unique collaboration mechanism was arranged. MIT in collaboration with INL, optimized the BISON settings for simulation of doped fuel. Then MIT turned in the BISON input files to FRAMATOME which has BISON license through CASL program. FRAMATOME then modified the inputfile with their proprietary boundary conditions for 3 different tests involving a power ramp. The results indicated a 15% underestimation of FGR by BISON, which is within the uncertainty of the code. In such way, we gained confidence in code prediction and capability for use in future projects while FRAMATOME kept its intellectual rights of its data.

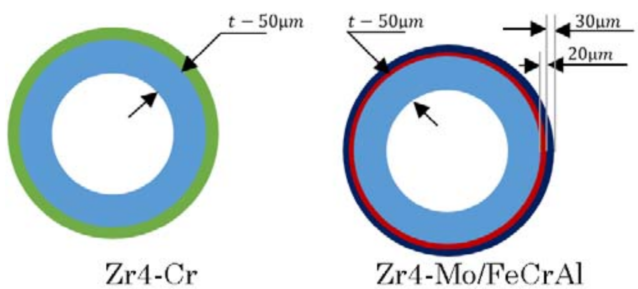


Figure 15. Different Zr4-based claddings and modeled coating thicknesses.

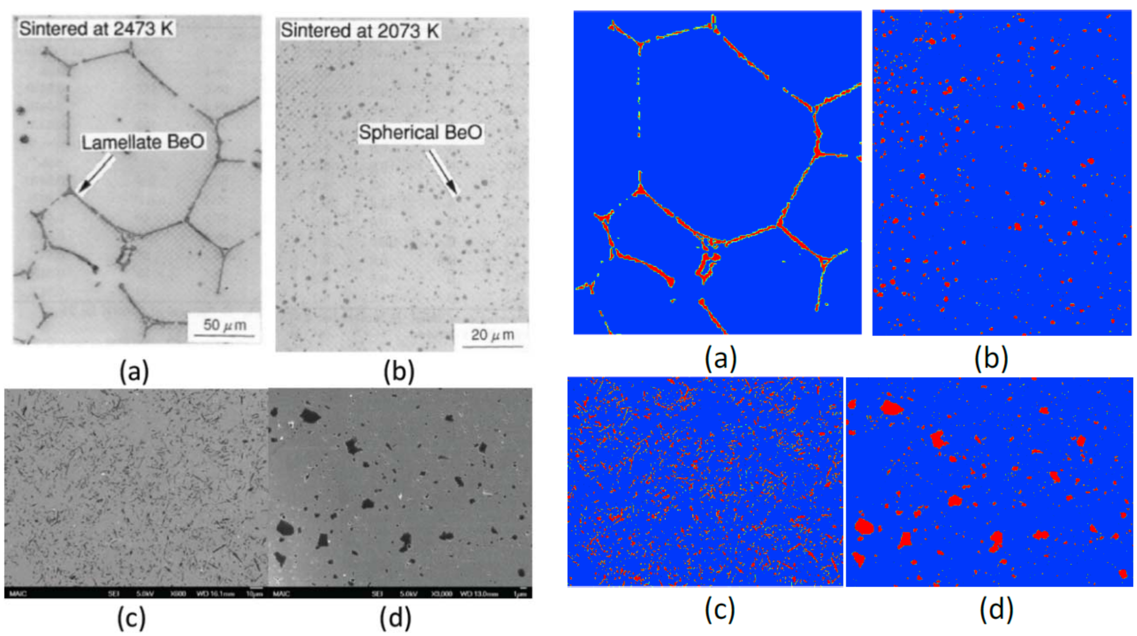


Figure 16. Microstructures obtained from literature (left) and reconstructed as part of this work (right), in all cases light phase is UO2 with dark phase being a high thermal conductivity additive. (a) Continuous BeO type from Ishimoto[15] (b) Dispersed BeO type from Ishimoto[15] (c) Dispersed SiC whiskers from Yeo[16] (d) Dispersed SiC particles from Yeo[16].

[15] Ishimoto S., Mutsumi H., Ito K., and Korei Y., *Journal of Nuclear Science and Technology* 33 (1996) 134-140.

[16] Yeo S., Mckenna E., Baney R., Subhash G., and Tulenko J., Journal of Nuclear Materials 433 (2013) 66-73.

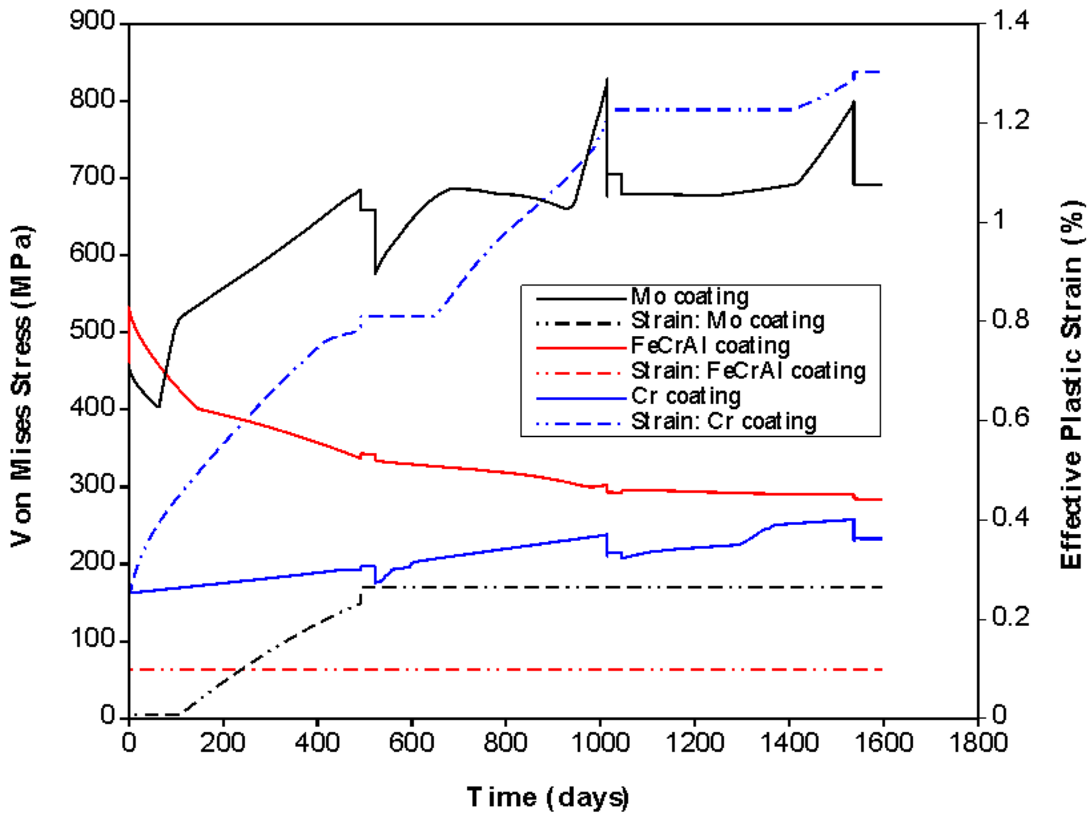


Figure 17. Stresses (solid) and effective plastic strains (dashed) in the different coating layers

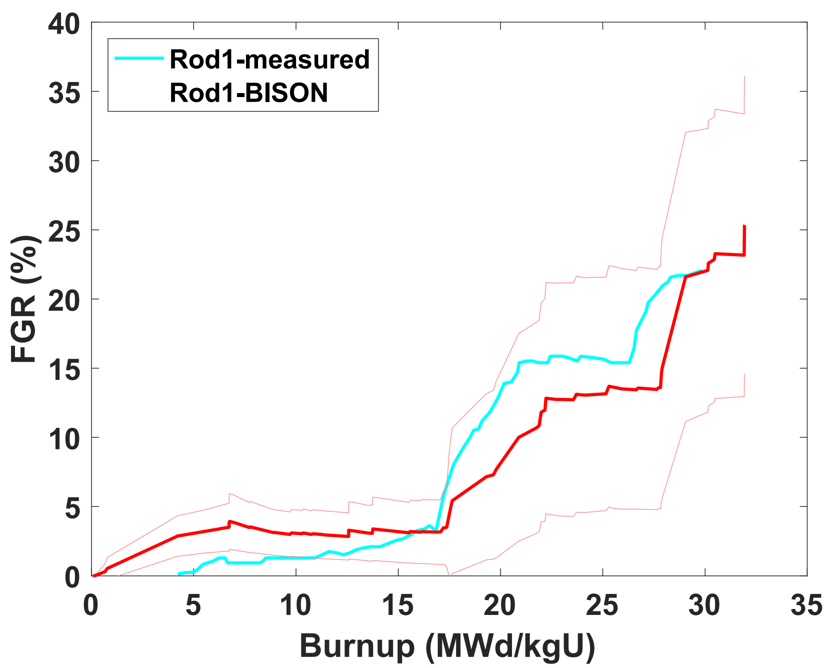


Figure 18. Time-dependent sensitivity analysis of fission gas release for the BISON simulation of IFA-677.1 rod 1 (The solid red line is the mean value of the FGR. The light red band is the ±σ uncertainty range. The solid line in cyan is the experimental FGR inferred from the rod pressure measurements).

Most of these findings on Cr-coating and doped fuel have been published in two articles, where more details are provided.[17,18]

The goal of the fuel with additive work was to use mesoscale simulations to inform the development of a macroscale model that predicts the thermal conductivity of UO_2 fuel with high thermal conductivity BeO and SiC powder and SiC whiskers additives. The 2D and 3D microstructure of these additives were reconstructed using the MOOSE framework. Additionally, a thermal resistor model was developed to predict the effective thermal conductivity of a composite material. This allows the developed computational models to be used as a material design tool by the nuclear community to optimize the gains in thermal-conductivity based on fuel design goals. Fig. 19 shows the thermal conductivity predictions for each microstructure shown in Fig. 16.

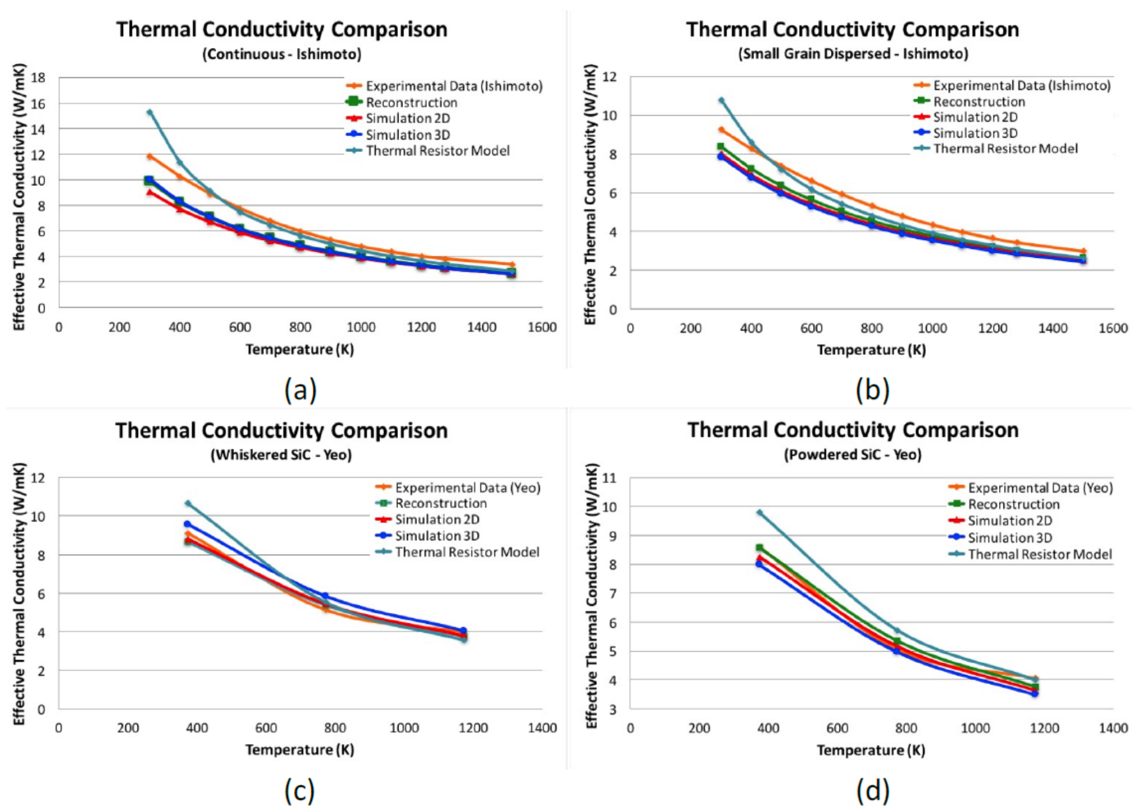


Figure 19. Thermal conductivity curves for each microstructure shown in Fig. 16. Note: In (a) the green reconstruction curve is obstructed by the blue 3D simulation line.

[17] Wagih, M., Spencer, B., Hales, J., Shirvan, K., *"Fuel performance of chromium-coated zirconium alloy and silicon carbide accident tolerant fuel claddings,"* Annals of Nuclear Energy, Vol 120, pp. 304-318, 2018.

[18] Che, Y., Pastore, G., Hales, J., Shirvan, K., "Modeling of Cr2O3-doped UO2as a near-term accident tolerant fuel for LWRs using the BISON code," Nuclear Engineering and Design, Vol 337 pp. 271-278, 2018.

2.8 Transient and Accident Fuel Performance Simulations of Near Term ATFs

The Accident Tolerant Fuel (ATF) program is focused on extending the time to fuel failure during postulated severe accidents compared to the standard UO_2-Zr alloy fuel system. To this end, we analyzed the transient and accident performance of selected near term ATF concepts (e.g. dopants/coatings):

1. Zr4-Chromium coated cladding (see Fig. 15) [Led by MIT and Structural Integrity (Formely known as ANATECH)]
2. Zr4-FeCrAl coated cladding with a molybdenum interlayer (see Fig. 15) [Led by MIT]
3. Chromia Doped Fuel (Large grain pellets) [Led by MIT and INL]

The coated claddings were kept to a ~50µm of coating thicknesses, deducted from the base layer thicknesses. The doped content were kept as found in literature for model validation. All three of the ATF concepts were studied, using MOOSE-based multi-physics fuel performance tool, BISON, under transient and accident PWR conditions in support of DOE AFC and NEAMs programs.

In this subsection, the transients considered were power ramps [Led by MIT] and load follow [Led by Structural Integrity (SI)]. The accident considered were Large Break LOCA [Led by MIT], Rod Ejection Accident [Led by SI]. The severe accident fuel mechanical performance was not modeled since to-date the NEAMS fuel performance tools lacks mature fracture mechanics and dynamic failure analysis capability for fuel engineering scale structural analysis during severe accidents.

The chromium coated concepts proved to be the most promising coated cladding concept, while the Zr4-Mo/FeCrAl cladding showed high plastic strains in the molybdenum layer relative to what Mo can handle, making its possibilities of survival questionable.

Interestingly, it was found that the buildup plasticity and stress in the coating during the normal operation as discussed in section 2.7, were higher than the ones observed during the power ramp study. This was due to the fact that the initial thermal expansion mismatch between the coating and Zr4 is the driving force behind the initial plasticity development. As the pellet comes in the contact with the cladding during the simulated power ramp, the imposed stress counters the thermal stress and relaxes the coating. The stress in Zr4 is also not worsen under any simulated case which is a critical findings in support of licensing of coated cladding.

In this study, a typical PWR fuel with zirconium alloy cladding and the concept of coated (25 and 50 microns of Cr layer) cladding in the simulated load follow condition were also modeled. The load follow study shows that the gap closure is slightly affected by the coating, but the PCI stress is comparable to the Zry cladding case, and very small decrease in the PCI stress is seen in the coated clad fuel due to the late gap closure of the fuels with coating cladding. Similar to the power ramp study, very small changes in the plastic strains are seen in the power cycles, although the effective plastic strain is ~1% at the end of life.

Due to thin thickness of the coating, during LOCA where the cladding undergoes ballooning, the coating goes under high plasticity. While the balloon size at burst was found to be slightly smaller for coated cladding concepts, the large plasticity observed may impact post burst oxidation performance of the cladding if the presence of the protective coating is taken credit for safety analysis.

During reactivity initiated accident (RIA) simulated as a rod ejection accident, the mismatch of thermal expansion between Cr and FeCrAl coating and Zry substrate during the cladding temperature escalation is also considered to be the main reason for development of the stress/strain, and irradiation hardening could exacerbate the response. A sensitivity study on the yield stress and thermal expansion coefficient was also performed and it has verified the impact of the thermal expansion on the cladding response. During the selected RIA case, the maximum plasticity predicted in hoop and axial direction in the coatings was on the same order as the Zry substrate.

Additionally, the power ramp tests of Cr_2O_3-doped UO_2 fuel rods were simulated with BISON, showing a satisfactory agreement of Fission Gas Release (FGR) predictions with the AREVA experimental database. Simulations captured the suppression of FGR relative to standard fuel, and the trend of a lower increase of FGR with increasing ramp terminal power level, confirming this advantage of Cr_2O_3-doped fuel over the conventional UO_2 fuel during power ramps. Finally, simulations of fuel behavior under during a LB-LOCA were performed. BISON predictions indicated that the fuel rod with Cr_2O_3-doped UO_2 was subject to a lower FGR and as a consequence, a reduced ballooning, less radioactive gas release upon fuel rod failure, and delayed fuel rod rupture compared to the fuel rod with standard UO_2. The magnitude of the improved performance in terms of FGR was found to be within the fuel performance prediction uncertainty. Below Figures 20-25 also summarize the major findings in this section.

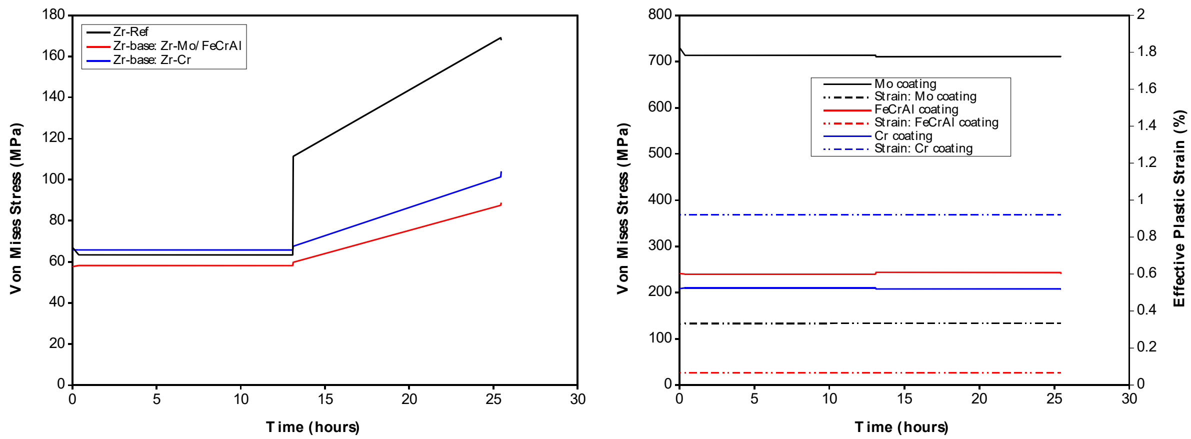


Figure 20. Von Misses (left) of base Zircaloy during simulated power ramp showing the coating will not increase the stress in the inner cladding; Von Misses (right-solid) and effective plastic strain (right-dashed) in the coatings during the power ramp showing that the steady state operation is as or more limiting as the power ramp for coating performance.

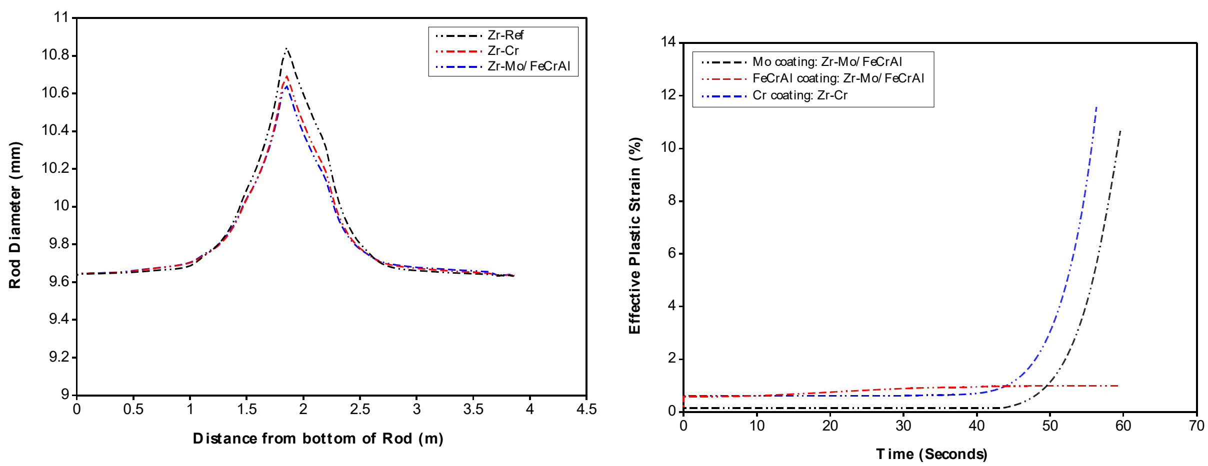
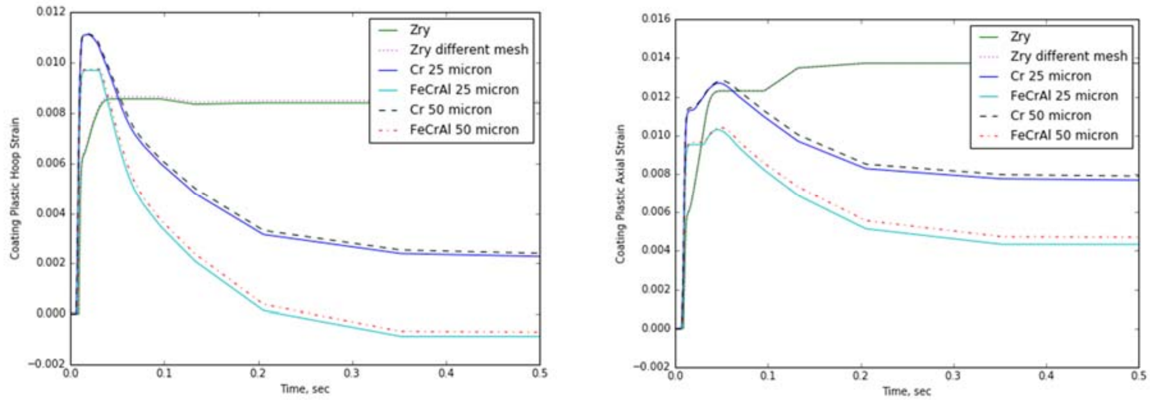


Figure 21. Ballooning (left) and effective plastic strain (right) of Zr and coated Zr cladding during a simulated LOCA. The results indicated minor change in ballooning size for the selected scenario and high plasticity near the balloon region due to small thickness of the coating.



(a) Plastic hoop strain (b) Plastic axial strain

Figure 22. Comparison of coating plastic strains for Zry, FeCrAl and Cr coating during RIA; Result indicate that while the evolution of stress/strain in the coating is different than Zry, the maximum magnitude reached is similar.

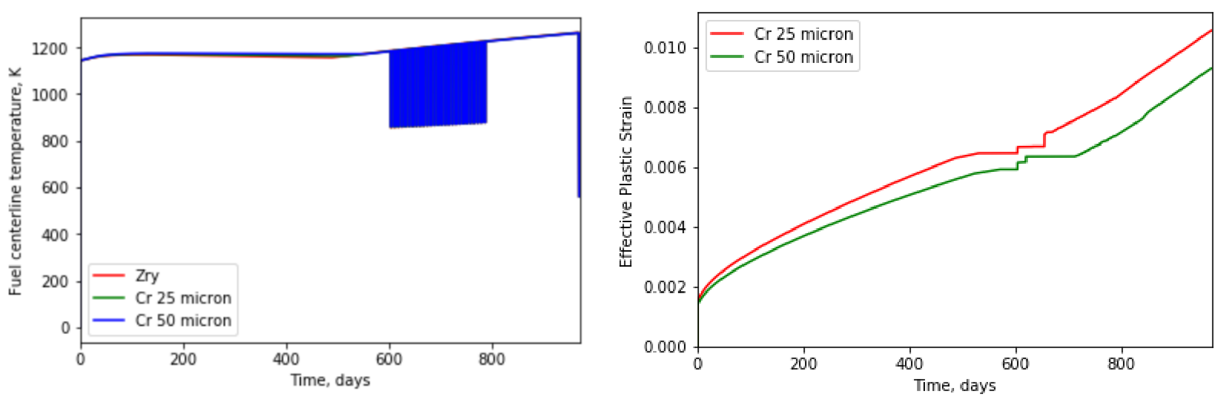


Figure 23. The fuel centerline temperature (left) and coating effective plastic strains (right) for different Cr coating thicknesses during a simulated load follow event.

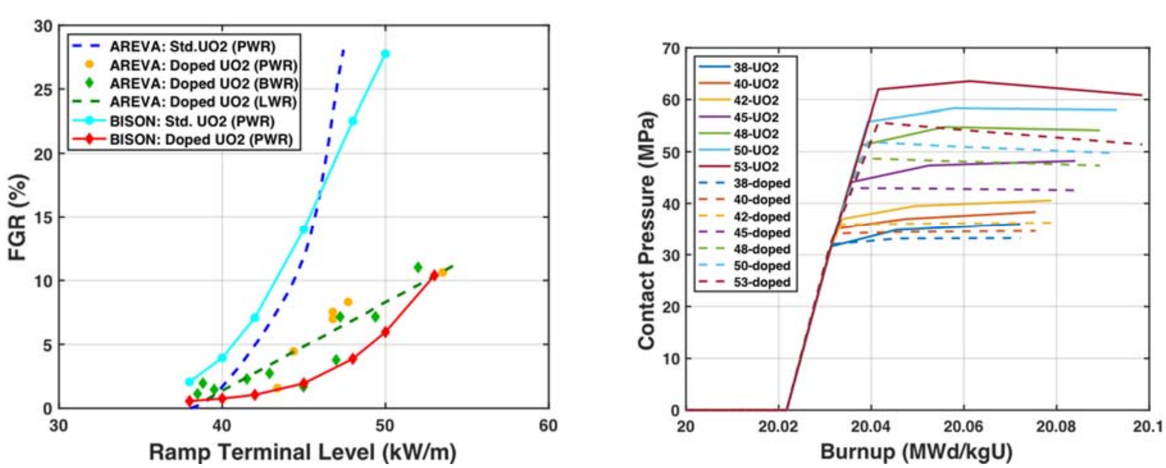


Figure 24. Fission gas release (left) and contact pressure (right) of Cr_2O_3-doped UO_2 fuel performance during power ramps. The result indicate lower fission gas release and softer contact consistent with in-pile experimental observations [Figures from Ref 18].

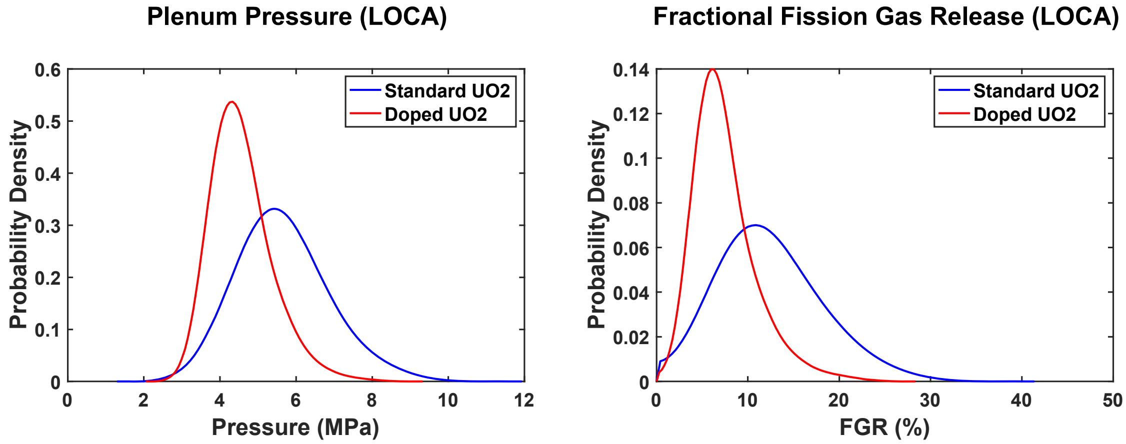


Figure 25. The probability density function of plenum pressure and fission gas release for doped and standard fuel during LOCA; Results indicate within uncertainty that the performance of doped fuel is superior to that of standard fuel.[19]

2.9 Economics and Cost Analysis

The main purpose of the effort in this section was to produce more comprehensive view of the impact of different coated material on fuel cost and overall safety performance of near term ATFs on plant economics. For the first objective using the reactor physics calculations presented in section 2.5, levelized fuel costs were calculated for different set of coated material (Cr vs. Mo/FeCrAl), coating thickness (20, 50 and 100 μm), spacer grid composition (Zr vs. FeCrAl) and fuel radius (reference vs. expand with coating thickness due to harder cladding) for both a PWR and a BWR assembly. The cost analysis assumed 10% interest rate.

For the second objective, the comprehensive view of existing plant systems were considered and role of ATF with respect to nuclear power plant economics was discussed. Specifically, the economic impact in terms of ATF implications to 50.69 safety-related classification, risk-informed 4b/5b programs to increase completion times to meet current tech spec limits and plant security and emergency planning zone boundary was overviewed. Since the goal of ATF is to substantially improve severe accident performance, the maintenance savings for reduction or removal of already installed FLEX equipment is also included in the discussion.

[19] Che Y., Wu X., Li W., Shirvan K., Pastore G., Hales J., *"Sensitivity and Uncertainty Analysis of Fuel Performance Assessment of Chromia-Doped Fuel During Large-Break LOCA,"* Topfuel, Prague Oct 2018.

For the fuel cost penalty from the coated material, our comprehensive analysis showed the importance of re-optimizing the fuel radius and considering a suitable spacer grid material to support economic deployment of near term ATFs. Cr coating thickness of 100 μm is equivalent to a coating thickness of 20 μm Mo with 20 μm FeCrAl, which results in increase of current fuel cost due to higher enrichment by ~4%. In addition, FeCrAl outer coating (or monolayer cladding) is not compatible with Zry spacer grids due to formation of low temperature eutectic and thus require FeCrAl spacer grids that increase the cost of fuel by additional 1% for PWRs. If the total cladding thickness is reduced by the coating thickness (i.e. if reference Zry cladding is 550 μm and the coating thickness is 50 μm then ATF cladding will be 500 μm – 450 μm Zry and 50 μm coating) and the fuel radius is increased, then the levelized fuel cost penalty due to existence of the coating is reduced by half. The reduction in total thickness of the cladding can be argued from the point of view of increased in strength of the cladding and reduction in the oxidation of the cladding from fuel performance point of view.

For the economic implications of ATFs, significant gain may be realized if sufficient cooling exists to ensure long coping time (~72 hours). Otherwise, as shown in section 2.6, the coping time from adoption of near term ATF alone will not increase significantly.

The primarily gain in economics (5-7% of the cost of electricity for an average nuclear power plant) is estimated to be from safety system reclassification. The current risk-informed program that industry is beginning to utilize is under 10CFR50.69. The original intent of 50.69 is to apply classification in terms of relative risk being "safety significant" and "not safety significant". It does not apply to absolute risk reduction. Thus, if an ATF cladding brings down the CDF and LERF in absolute terms, then the classification of the components involved in the accident sequences contributing to CDF and LERF may not be impacted. Thus, ATF application for 50.69 requires regulatory approval to apply classification on absolute risk limits basis and so, economic savings is highly uncertain.[20]

Cost savings from mitigation of fuel leakers and TMI type accidents are likely not significant due to the low probability of failure of conventional UO2/Zr fuel and intensive operator training of existing fleet since the TMI accident, respectively.

[20] Shirvan K., Grantom C.R., "Risk Implications of Using Accident Tolerant Fuels in LWRs," Probability Safety Assessment Conference (PSA), Pittsburg, Sept. 2017

2.10 Time to Fuel Failure Analysis

The aim of Multiphysics analysis is to more accurately determine the performance of a nuclear reactor core. The focus of this task was to integrate reactor physics, thermal hydraulics and fuel performance informed by the coated clad experimental data in an integrated framework for accurate estimation of time-to-failure (beyond design basis accident) for near term ATF concepts. Section 2.5 major finding showed that the reactor physics performance of coated cladding is very similar to UO2/Zr system and thus there was no need to integrate such physics as current experience implies a weak coupling for safety performance of LWRs and traditional tools have sufficient capability. For thermal-hydraulics we chose system code TRACE due to availability of source code and lack of readiness of NEAMS's RELAP7. TRACE already integrates limited fuel performance capability within the code including burnup dependent strains, ballooning, burst and oxidation. The NEAMS tool, BISON can provide more resolution of nuclear fuel performance. However, BISON does not have the capability to move to beyond design basis accident to estimate time-to-failure as the simulation ends at burst. Thus, we built more detailed fuel performance models within TRACE including the ATF material models. We extended the analysis capability shown in section 2.6 by allowing TRACE to continue to simulate reactor thermal-hydraulics after melting point of any material has reached and stop the simulation at the time where all cladding has been oxidized. The current simulation temperature limit for the near term fuel concepts is limited to UO2/Zr eutectic temperature, consistent with MELCOR. As such we are able to more accurately capture time-to-failure of the different fuel concepts and meet our original objective by utilizing a modified TRACE executable.

Consistent with the major findings found in section 2.6, it was found that the amount of hydrogen generated during a severe accident is strongly correlated to the cladding thickness relative to oxidation of non-fuel material or cladding material. Section 2.6 only overviewed PWR findings, in this section we also created a reference BWR model in TRACE. For BWR, the channel box did generate substantially higher hydrogen mass than the guide tubes and control rods in a PWR. Nevertheless, for figure-of-merit of time-to-fuel melt, this hydrogen generation from channel box was significantly lower than the fuel cladding. The following are more specific conclusions regarding the BWR model which is also consistent with the PWR model.

1. The reduction in time to melt by ATF claddings ranges from 1 minute to 20 minutes, and it is longer for slower transients (Short vs. Long term SBO). Therefore the gain in coping time by these

near-term claddings are only marginal. It should be noted that the heat up rate predicted by TRACE is much faster than MELCOR and the specific reason behind this difference are still unknown.

2. The hydrogen generated by the cladding material at the time of cladding melt is significantly reduced with ATF claddings. At the time of complete cladding oxidation, the hydrogen generated by Cr-coated cladding is similar to Zircaloy, while those generated by FeCrAl claddings are reduced by 42% - 47%.

3. The hydrogen gas generated by FeCrAl channel box at the end of simulation is only slightly lower than those by Zircaloy. The reason is that FeCrAl channel box reacts faster with high temperature steam. By the time of cladding fully oxidizes, more FeCrAl channel box is reacted than Zircaloy. Therefore if the simulation continues using severe accident codes, the reduction in hydrogen gas generation by FeCrAl channel box will be more obvious.

4. FeCrAl-ORNL case generally has less hydrogen gas generated than the FeCrAl-MIT cases. The reason is that FeCrAl-ORNL channel wall switches from aluminum oxidation to iron oxidation at 1775 K while the transition temperature for FeCrAl-MIT is 1640 K. Both oxidation models are threshold reactions but the iron oxidation is more catastrophic.

The ATF program was mandated by congress in search of fuels with superior severe accident performance. In this IRP, the system code TRACE predicts up to 20 minutes added coping time while MELCOR simulations predicts up to 2 hours for station blackout type scenarios. In either case, the capacity to provide additional core cooling as an alternative severe accident mitigation strategy is deemed to be more effective for existing plants. However, outside of their modest coping time improvements, ATFs do present other safety and economic opportunities in form of more resilient fuel for normal operation and design basis accidents and have potential to enable higher fuel burnups. In order to realize such benefits, significant R&D is needed to address new failure modes and build the safety and commercial case. These challenges can be overcome through a public-private partnership between the DOE and industry.

3. Recommended Future Work

In this section, the recommended future work is presented. First, future ATF-themed NEUP topics are recommended in terms of each industrial ATF concept. Then future work in context of what was originally planned in the IRP but was not accomplished is discussed. Finally, other recommended future work driven by the major findings are included in this section.

3.1 Recommended NEUP Direction on ATF

1. Coated Cladding: Fundamental study on fatigue performance with irradiation damage in terms of coating process parameter on Zircaloy is highly recommended. For the irradiation damage, unless an NSUF for HFIR or ATR is possible, the focus should be on ion irradiation given that NEUP's are university led projects where either high energy protons or Cr-based beam is utilized to obtain representative performance. The scope of work should cover both Cold-spray and PVD coating processes and include both metallic Cr and ceramic CrN to remain industry relevant. This work will address the fundamental failure mode that the industry will have to prove to the regulator during the coated clad licensing process.
2. Doped fuel: The fission gas release has already been or current being addressed through multiple projects and avenues. What is needed in the future is fundamental modeling of the PCMI for Doped fuel and Zircaloy cladding. The understanding of PCMI and fuel mechanical structure is important for high burnup fuel, thus the recommended future work should be focused on developing surrogate testing procedure and meso-scale modeling to emulate a high burnup doped fuel. Otherwise, for fresh fuel, such study is of minimum value.
3. SiC/SiC cladding: Beyond existing and planned work, the explicit PCMI testing of SiC composite cladding under prototypic conditions with both UO_2 and high density fuels (U3Si2/UN) is of high interest and currently not covered by any funded programs. The degree of PCMI will determine the viability of the concept. Both out-of-pile and in-pile testing are recommended for future work. Particularly in case of SiC cladding, since its swelling saturates at low dpa, an in-pile testing as a university-led project is possible.
4. High Density Fuels (U3Si2/UN): Closer collaboration with Universities on hydrothermal corrosion of high density fuels including mitigating actions are recommended. The fission gas release and swelling of these fuels vs. burnup are still highly uncertain. The preliminary lower

scale modeling predicted the opposite trend than measured in the ATR for U_3Si_2 fuel as part of ATF-1 test campaign. Revisiting such efforts given the current state of knowledge augmented with initial data from ATR would be a worthwhile university-led project.

5. Fuel performance for beyond design basis: This is an area were academic leadership is needed as it will likely become important to industry in the near future. Through our experimental program of this project, multiple new failure modes were identified for ATF concepts. For instances, buckling/bending of cladding due to lack of presence of thick oxide layer that would prevent mitigation action in a severe accident. Such failure mode/scenario is postulated to be worse for FeCrAl cladding vs. Cr-coated cladding where a bond between the fuel and cladding is not expected and the cladding could "slide off" the fuel. With currently accepted regulatory guide on "mechanistic source term", it is of interest to tackle such failure modes including fuel collapse through a modeling and simulation framework instead of coarse empirical approaches based on static temperature.
6. Post Critical Heat Flux (Post-CHF) Heat Transfer Regime: In order to utilize ATF concept to their maximum potential, post critical heat flux heat transfer regime needs to be experimentally and computationally characterized. Despite all the current focus on CHF, what will become more important is Post-CHF heat transfer regime for utilities and vendors. The ability of ATF concepts to potentially survive after CHF will depend on post CHF heat transfer efficiency and is an important area of future work and could be significant part of ATF value proposition.

3.2 Recommended Work not Accomplished by the IRP

1. As recommended in the previous section (item 5 in section 3.1), fuel performance during sever accident was not explicitly address though a structural mechanics framework as originally intended. The system code simulations indicated that cladding melting point for near term ATF concepts is reached in similar time range as Zircaloy. Thus, there was little incentive to spend major effort for simulation on this front given the lack of relevant mature capability in MOOSE framework. While non-fuel core component behavior was found to be not important in the safety assessment, the exact mode of fuel collapse may allow reduction in conservatism and contribute to the current accepted mechanistic source term methodology. This work would be of interest in the future for long term ATFs as well as introduction of FLEX type strategies

combined with near term ATF were the coping time could be extended and such modeling effort would have higher impact.

2. Atomistic and meso-sclae modeling of corrosion and inter-layer interaction for coated cladding was not addressed in the IRP as originally intended. The main reason this was not addressed in the IRP was re-prioritization of the effort on producing critical data on failure modes. This is still an area of scientific interest that can help the ATF campaign to fundamentally better understand the mechanism behind coated clad performance (partially addressed by Item 1 in Section 3.1) given much data is not available.
3. Coupling of NEAMS MOOSE-based tools for multiphysics analysis of ATF concepts was not explicitly addressed as originally intended. As stated in the original proposal, Rattlesnake was planned to be used for reactor physics calculations. However, the reactor physics implication of the consider ATF concepts proved to result in marginal difference relative to Zircaloy and thus there was no need to utilize such non-commercial tool. For more exotic ATF concepts outside of the vendor concepts, such as FCM or Lightbridge metallic fuel, the use of rattlesnake may be more appropriate. It was originally stated that if RELAP7 is ready, it would have been used for the system code predictions instead of TRACE. However, at the end of the IRP, RELAP7 continues to be under development phase and not in use for ATF safety predictions. If RELAP7 becomes available in near future, its use would be of interest for ATF predictions to demonstrate its attributes. Lastly, the coupling of the codes, RATTLESNAKE, RELAP7 and BISON were not pursued. This was due to the uncoupled nature of near term ATFs during severe accident conditions. Perhaps for more exotic ATF concepts such as FCM and metallic Lightbridge fuel, this work would be of interest.
4. MAX phase alloys were not pursued as a coating concept as originally intended since their radiation instability was highlighted through multiple irradiation campaigns at the start of the IRP. Cr metal with its diffusion and formation of eutectic and CrN ceramic with its decomposition concerns still motivates a search for a MAX-type alloy that is radiation resistance. Such search may still be of interest in the future to maximize the economic value of the coated clad ATF concept.
5. In the proposal, originally, we promised to perform a code-to-code comparison of FALCON fuel performance code to BISON for different near term ATF concepts. However, this work was not performed since EPRI, who holds license for FALCON, did not allow Structural

Integrity, the developer of the FALCON code, to use it for this IRP. Code-to-code comparisons are key in further enhancing of NEAMS tools and DOE should find ways to support such activities in the future.

3.3 Other Recommended Future work

For coated cladding experimental testing:

1. Prototypic grid-to-rod wear testing to ensure the structural integrity of Zircaloy grids to address both regulatory limits (channel blockage/coolable geometry) and operational limits (fuel handling). Out-of-pile testing is likely sufficient.
2. Standard burst testing on the final product to ensure ballooning and burst area are similar or lower than Zircaloy. Out-of-pile testing is likely sufficient.
3. Fatigue mechanical/thermal cycling testing to ensure the coating adhesion and similar or improved crack propagation compared to Zircaloy in order to address concerns regarding fuel washout behavior and post-failed rod fuel handling. Current, Zircaloy fatigue design basis by O'Donnell and Langer is a good starting point.
4. Integral neutron irradiated fuel test (UO2/Zr/Cr-coating) in prototypic coolant chemistry environment to address the primary concerns with coating adhesion, irradiation induced swelling, local hydriding and geometry specification (including tolerances). It is recommended that some tests be performed purposely with defective coating to alleviate any concerns in these areas.
5. Destructive or Non-destructive examination (NDE) qualification techniques of coating inspection needs to be developed to show that coating meets the geometric specifications within the specified tolerances before insertion and coating has survived after irradiation.
6. Severe accident demonstration of coated cladding may be needed to ensure similar failure mode is observed as Zircaloy cladding. Severe accident modeling could be first utilized to perform bounding analysis to determine if such testing will be needed given current plant severe accident requirements and performance.

For Improvement of NEAMS fuel performance tool BISON for Transients and Design Basis Accidents:

1. Current material property models for coated cladding used in the evaluation are largely based on open literature data and very few irradiated data is available for Chromium as metal or coating.

Update of those material models is necessary if new data can be generated from experimental programs. Since the LTRs and LTAs will not take any structural credit for the coating, the generation of these data is of high interest for the end-use of the coated cladding concepts rather than LTRs and LTAs.

2. Current modeling approach meshes coating as a separate layer; this would make the modeling under radial-axisymmetric geometry more challenging for the commercial nuclear fuel, considering its long fuel length, and high aspect ratio in finite element meshing. Alternatively, different modeling approach should be pursued to make the coating mesh more robust and scalable. Some issues with regard to the responses of coated cladding with flaws, e.g. the delamination, wear marks and/or cracking of the coating layer, were not studied. Preliminary attempts were made and meshing scripts has been written to automate the defect formations. Due to high aspect ratios, significant convergence issues were faced during simulations. A combine simulation/experiment approach in improving our understanding of coated cladding defects and its evolution is recommended for future work and area of high priority.

3. The simulated LOCA in this milestone had fast heat-up rate. Cr-coated cladding have shown to have significantly lower balloon size and burst size with slower high temperature creep tests. It is unclear whether the implemented models will be able to capture such phenomena. The initial attempt to capture such phenomena was not successful due to numerical divergence of the code. This is an area of priority and scientific interest for future modeling work. In addition, it was found that the pre-oxidation burst stress model in BISON gives unrealistic results and more validation is required in this area.

4. For doped fuel, the investigation of the difference in fuel cracking and its implication on PCMI and fuel washout behavior post-burst is reserved for future work. In general, it is recommended for DOE programs to continue support BISON's PCMI modeling development as many convergence issues were faced with the most up-to-date version of the BISON fuel performance code.

For improvement of TRACE Severe accident simulations:

1. The BWR compartments (Drywell and Wetwell) in TRACE containment are homogeneous volumes that cannot account for non-uniformities in the temperature. Therefore, the quantitative containment responses during BDBA simulations using TRACE is limited compared with

MELCOR simulations [USNRC, 2012-SOARCA-BWR] which can divide the Drywell compartment into multiple connected volumes to model the non-uniformities.

2. Sensitivity and uncertainty analysis for the major FOMs for various BDBA scenarios. The oxidation models are highly uncertain because they are empirical models fitted based on limited set of HTSO experiments.

3. A previous work [Mandelli, et al., 2016-NT] performed stochastic analysis following the Risk-Informed Safety Margin Characterization (RISMC) pathway to evaluate the impact of power uprate on a BWR SBO accident scenario. Twelve parameters related to SBO simulation were considered as uncertain, such as battery failure time, batter life, Firewater flow rate, etc. In the future, we will perform similar stochastic analysis using uncertain parameters that are available in this particular BWR model.

4. Containment heat structure and SP liquid cooling system were not considered in this study.

5. Heat loss from the vessel to the containment was not considered in this study.

6. The current oxidation model is not function of available oxygen next to the cladding, thus oxidation maybe over estimated.

For improvement in ATF value proposition:

1. The fuel levelized cost estimation in this study ignored the fabrication cost of the coating. Currently, the industry fuel vendors use different techniques for fabrication of the coating on Zry cladding. Much like with similar processes, the cost for mass production of the coated clad is currently highly uncertain. However, attempts should be made to include such estimates.

2. Significant economic gain was estimated to be realized through substantial increase in coping time and better radionuclide retention. Since ATF alone will not be able to provide such benefits, additional coupling to other safety systems should be explored and the economic implication should be quantified. Currently, there are DOE funded projects at labs and universities that are working on this front as part of the LWR sustainability program including the MIT and Wisconsin teams from this IRP.

4. Published Journal Articles

1. J., Wang, M., Mccabe, M.L., Corradini, et al., *"Accident tolerant clad material modeling by MELCOR: benchmark for SURRY short term station blackout"*, Nuclear Engineering and Design, 313, 458-469, March 2017
2. Sevecek M., Gurgen A., Seshadri A., Che Y., Wagih M., Phillips B., Champagne V, Shirvan K., *"Development of Cr Cold-Sprayed Fuel Cladding with Enhanced Accident Tolerance,"* Nuclear Engineering and Technology Journal, Vol 50, pp. 229-236, 2018.
3. Deng, Y., Shirvan, K., Wu, Y., Su, G. "Probabilistic view of SiC/SiC composite cladding failure based on full core thermo-mechanical response," Journal of Nuclear Materials, Vol 507, pp. 24-37, 2018.
4. Seshadri A., Philips B., Shirvan K., *"Towards Understanding the Effects of Irradiation on Quenching Heat Transfer,"* Journal of Heat and Mass Transfer, Vol 127 pp. 1087-1095, 2018.
5. Seshadri A., Shirvan K., *"Quenching Heat Transfer Analysis of Accident Tolerant Coated Fuel Cladding,"* Nuclear Engineering and Design, Vol. 338 pp. 5-15, 2018.
6. Capps N., Mai A., Kennard M., Liu W., *"PCI analysis of Zircaloy coated clad under LWR steady state and reactor startup operations using BISON fuel performance code,"* Nuclear Engineering and Design, Vol 332 pp. 383-391, 2018.
7. Wagih, M., Spencer, B., Hales, J., Shirvan, K., *"Fuel performance of chromium-coated zirconium alloy and silicon carbide accident tolerant fuel claddings,"* Annals of Nuclear Energy, Vol 120, pp. 304-318, 2018.
8. Che, Y., Pastore, G., Hales, J., Shirvan, K., *"Modeling of Cr2O3-doped UO2as a near-term accident tolerant fuel for LWRs using the BISON code,"* Nuclear Engineering and Design, Vol 337 pp. 271-278, 2018.
9. Gurgen, A., Shirvan, K., "*Estimation of coping time in pressurized water reactors for near term accident tolerant fuel claddings"*, Nuclear Engineering and Design, Vol 337 pp. 38-50, 2018.
10. J., Wang, M., Mccabe, T.C., Haskin, et al., "*Iron-chromium-aluminum (FeCrAl) cladding oxidation kinetics and auxiliary feedwater sensitivity analysis: short-term station blackout simulation of Surry nuclear power plant"*, ASME Journal of Nuclear Engineering and Radiation Science, 4 (4), 041002: 1-9, September 10, 2018.
11. J., Wang, H.J., Jo, M.L., Corradini, et al., *"Potential recovery actions from a severe accident in a PWR: MELCOR analysis of a station blackout scenario"*, Nuclear Technology, 240 (1), 1-14, 2018.
12. Gigax J., G., Kennas M., Kim H., Maier B., Yeom H., Johnson G., Sridharan K., Shao L., *"Interface reactions and mechanical properties of FeCrAl-coated Zircaloy-4,"* Journal of Nuclear Materials, Vol 519, P. 57-63, 2019.

Appendix A

White Paper on Experimental and Testing Needs for Deployment of Chromium Coated Cladding

Koroush Shirvan
Department of Nuclear Science and Engineering
Massachusetts Institute of Technology

Kumar Sridharan
Greg Johnson and Tyler Dabney
Department of Engineering Physics
University of Wisconsin-Madison

Disclaimer
The following represents only the views of the first author with supporting contributions from the other co-authors and Michael Corradini of University of Wisconsin-Madison, Chris Lewis and Kiran Nimishakawi of Framatome. No rigorous peer-review has been done on corroborating the accuracy of the statements and recommendations of the content as it should be treated as a white paper aiming to better inform accident tolerant fuel deployment and future R&D directions.

Summary
The following white paper discusses the experimental and testing needs for deployment of Chromium (Cr) coated cladding technology in light water reactors. It is important to note that the discussion is focused on current licensing requirements (NRC-view) and current operational limits (Utility-view) for Cr-coating WITHOUT taking into credit any of its benefits. In another words, the discussion is only on how the coating would impact the existing licensing limit and existing practice in fuel reload and operation. A brief discussion is included at the end of the white paper on R&D needs to realize higher peak clad temperature (PCT) and higher burnup limits by using the coating to improve LWR economics.
The following testing summarizes the gaps identified in this paper.

1. Prototypic grid-to-rod wear testing to ensure the structural integrity of Zircaloy grids to address both regulatory limits (channel blockage/coolable geometry) and operational limits (fuel handling). Out-of-pile testing is likely sufficient.
2. Standard burst testing on the final product to ensure ballooning and burst area are similar or lower than Zircaloy. Out-of-pile testing is likely sufficient.
3. Fatigue mechanical/thermal cycling testing to ensure the coating adhesion and similar or improved crack propagation compared to Zircaloy in order to address concerns regarding fuel washout behavior and post-failed rod fuel handling. Current, Zircaloy fatigue design basis by O'Donnell and Langer is a good starting point.
4. Integral neutron irradiated fuel test (UO_2/Zr/Cr-coating) in prototypic coolant chemistry environment to address the primary concerns with coating adhesion, irradiation induced swelling, local hydriding and geometry specification (including tolerances). It is recommended that some tests be performed purposely with defective coating to alleviate any concerns in these areas. The target burnup of such integral test can either be ~30

MWd/kgU to support initial reload licensing or ~60 MWd/kgU for eventual full core deployment, depending on the Utility's level of risk acceptance and NRC licensing requirements. Post-irradiation will include hydrogen extraction and mechanical testing (such as ring-compression) to ensure cladding ductility is preserved with the coating and defective coating. Loss of Coolant Accident (LOCA) testing is also recommended to ensure burst area gives acceptable performance.

5. Destructive or Non-destructive examination (NDE) qualification techniques of coating inspection needs to be developed to show that coating meets the geometric specifications within the specified tolerances before insertion and coating has survived after irradiation.
6. Severe accident demonstration of coated cladding may be needed to ensure similar failure mode is observed as Zircaloy cladding. Severe accident modeling could be first utilized to perform bounding analysis to determine if such testing will be needed given current plant severe accident requirements and performance.

Addressing the above items will depend on fabrication technique and coating thickness, thus each vendor have to perform their own tests. The most time and cost intensive item is number 4 for which physics-based rational could be made such that reliance on down scaled and accelerated neutron testing maybe allowable. An example of such test are the planned rodlets to be irradiated at the Advance Test Reactor PWR loop in Idaho National Laboratory to address primary concerns with coating adhesion, irradiation induced swelling, local hydriding and geometry specification (including tolerances). Thus, LTR and LTA programs in nuclear reactors will serve to give additional confirmatory confidence (which is still needed) to the performance of the rods as majority of the destructive and time sensitive testing could be done in an accelerated environment such as ATR on a scaled rod geometry. While, extensive prototypic full scale data on coating performance along with separate effect tests on Cr and Cr-coating thermo-mechanical properties are "nice to have", given the overall expected minor impact of the coating on the performance of fuel/cladding, it is not envisioned extensive testing would be needed beyond what is recommended to meet current regulatory limits and operational practices with UO_2/Zr fuel.

R&D Areas of Interest

TEST	*NEED*	*REASON*	*COMMENT*
REACTOR PHYSICS:	None	Insignificant Impact	10-30 um thickness makes insignificant impact [REF]
THERMAL HYDRAULICS/SAFETY			
THERMAL PROPERTIES	None	Insignificant Impact	Data for Cr is available up to 1000 C [REF]; 10-30 um will not make significant difference given expected properties [REF]
MECHANICAL PROPERTIES	None	Insignificant Impact	10-30 um Coating will not play a structural role in the cladding [REF]; Mechanical tests (Ring Compression) should be done on the final product for verification. Integral validation of coated clad at high burnup is also sufficient vs. separate effect of mechanical properties (nice to have for future).
ROUGHNESS	None	Insignificant Change	Vendors have demonstrated ability to fabricate coatings with specified surface morphology [REF]
ADHESION EFFECTS	Yes	Gross Delamination (Operational and Regulatory Issue)	Complete delamination of 10-30 um coating could lead to fretting, three-body debris failure, CRUD Induced Localized Corrosion (CILC), Sress Corrosion Cracking (SCC) for normal operation and flow blockage during accidents; Low burnup data available [REF]; Need: High Burnup Data; Ion Irradiation has been performed and underway [Not publically available]; ATR/HFIR Irradiation could be utilized; Relevant Standards: ASTM B571-18, ASTM C633-13, ISO 14188:2012, ASTM C1525-18
PHASE CHANGE/INTERACTION	None	Compatible Materials	Thermal diffusion of Cr in Zr at low temperature is very slow; no significant phase formation that would degrade Zr or steel material structural integrity present in the core (including control rods) is expected for postulated accidents [REF]
OXIDATION RATE/MECHANISM	None	Positive Impact	Chromia is a single phase oxide and cr-coating oxidation performance has been repeatedly shown in open literature to be significantly lower than Zr [REF, REF, REF]; Heat of reaction for Cr to Cr_2O_3 is also lower than Zr [REF]

HYDROGEN PICKUP	Yes	Hydriding (Operational Issue; May require regulatory guidance)	Coating may prevent formation of passive ZrO_2 and/or allow for formation of local hydrides at defect locations due to stress/oxide presence; Limited testing has been done in open literature [REF], therefore more comprehensive testing should be done at high burnup. Such H pickup will be dependent on coating fabrication technique and its Zry substrate.
BURST CRITERIA/BLOCKAGE	Yes	Regulatory limit (Expected to be non-issue)	Diffusion of hydrogen from water through coating and hydrogen associated with the formation of chromia; Pre-irradiation ballooning is typically most limited, however, lack of pre-oxidation could result in different burst at higher burnup; limited testing has been done in open literature [REF], more comprehensive testing is needed. Such burst will be dependent on coating fabrication technique and the type of Zr-aloy substrate.
TMIN/REWET TEMP	None	Insignificant Impact (May require regulatory guidance)	Data for Cr in open literature suggests minor changes to surface properties and chemistry. The reduction in heat of reaction of Cr will further reduce any concerns [REF]; NRC staff guidance will dictate future testing needs.
CRITICAL HEAT FLUX	None	Insignificant Impact (May require regulatory guidance)	Vendors will aim to maintain similar surface roughness as Zircaloy; Effect of surface chemistry are expected to be low [REF]; Current data base is based on Inconel: Single rod prototypic out-of-pile testing is being currently performed as part of DOE ATF program. Testing will also give insights in coating adhesion post-CHF.
CRUD ADHERENCE (CIPS/CILC)	Yes	Operational Limit	Theory to predict CRUD deposition is weak so need data to verify that there will be no expected changes; Limited data collected at MIT (not published) implies non-issue.
GEOMETRY SPECIFICATION	Yes	Quality Assurance	Vendors need to demonstrate examination techniques (destructive or non-destructive) to verify the uniformity of the coating and presence of defects within reason.
EMISSIVITY	Yes	Safety Analysis Input	Limited data collected at MIT [REF]; Emissivity is needed as input for the safety analysis.

FUEL PERFORMANCE			
PCI (INCLUDING MECHANICAL/CHEMICAL AND PRESENCE OF HBS)	None	Insignificant Impact	Analysis in open literature suggests 10-30 um coating will not change the integrity of Zircaloy [REF] as expected.
CORROSION	None	Positive Impact	Data shows corrosion will be reduced [REF, REF, REF]
RADIATION INDUCED SEGREGATION/MIXING	None	Insignificant Impact	While data will be welcomed, impact is expected to be minimal due to thickness of the considered coatings (10-30 um)
CLAD PLASTICITY LIMITS	None	Insignificant Impact	Analysis in open literature suggests 10-30 um coating will not change the integrity of Zircaloy [REF]
COOLABLE GEOMETRY	Yes	Regulatory limit	Coating thickness needs to meet licensed/design tolerances (e.g. If coating is on top of existing cladding at 30 um then ~1/3 of hoop strain limit is already used up). Limited data on ballooning available [REF] but more comprehensive data base is needed.
FUEL WASH OUT BEHAVIOR	Yes	Regulatory limit	Burst size needs to be measured through comprehensive testing to ensure it is smaller or the same. Current data are encouraging [REF].
FATIGUE/AGING/CRACK PROPAGATION	Yes	Local Defects	Coating adhesion may become compromised with cyclic loading (similar to adhesion concerns). Coating may result in accelerated crack propagation due to hardness, fabrication technique, etc.; limited accelerated testing has been done in open literature [REF], more comprehensive testing is needed. Current, Zircaloy fatigue design basis is a good starting point [REF]
CREEP (MECH,THERMAL,IRRADIATION)	None	Insignificant Impact	Integral validation (coating with cladding) at high burnup is sufficient enough vs. separate effect coating properties (nice to have in future) for a given thickness.
SWELLING	Yes	Regulatory limit	Expected to be small but no data on high neutron DPA on coatings on Zr is available; Ion irradiation (not published) hint that swelling will be small but non-negligible.
COOLANT CHEMISTRY EFFECTS	None	Insignificant Impact	Cr is already part of most of reactor piping and structures [REF]
TRITIUM PERMEABILITY	Yes	Operational Limit	Lack of ZrO_2 and presence of small Cr_2O_3 motivates checking the tritium leakage of Cr-coated rod; Depends on fabrication technique and thickness.
FUEL ROD-GRID INTERACTION	Yes	Operational Limit	Limited data collected in open literature suggests an improvement in wear

			capability of the rod [REF], similar data needs to show that the grids themselves will remain intact in long term.
SEVERE ACCIDENTS			
PHASE CHANGE/INTERACTION	Yes	SA Analysis Input	Limited data collected in open literature do not show any significant impact of the eutectic formed between Zr/Cr at ~1330 C on structural integrity of the rod [REF]. One concern could be a more rapid hydrogen generation of the coating when >1330 ^{o}C due to absence of the protective ZrO2 layer. Other core materials are made of Zr or steel, so no unknown phase interactions are expected.
FAILURE MODE (ZIPPING/BOWING)	Yes	SA Analysis Input	Limited data at MIT on rodlets show that in severe accident domain fuel may undergoes zipping or significant bowing [REF,REF]. Such implication on severe accident progression and source term needs to be addressed; Expected to have minimal impact. Failure mode will depend on coating fabrication technique and thickness as well as underlying Zry substrate.
PRAS	Yes	Above is an input	As long as the above two items under severe accidents are shown to have acceptable performance then there will be no change required in plant PRAs with coatings. In general, improved oxidation kinetics could improve coping times (reduced metal/water reaction) that in turn could lead to delayed rupture of cladding leading to improved CDF and LERF.
FRONTEND			
TRANSPORTATION REQUIREMENT	None	Insignificant Impact	Fuel ductility is maintained while hardness is increased with the coating [REF]
INSPECTION	Yes	Quality Assurance	Vendors need to demonstrate examination techniques (destructive or non-destructive) to verify the uniformity of the coating and presence of defects within reason.
BACKEND			
TRANSPORTATION REQUIREMENT	Yes	Operational Limit	Overall fuel ductility and hardness is expected to improve but the concerns raised previously on “local hydriding” and “Fatigue” needs to be addressed

OPERATIONAL DOSE/ACTIVATION	Yes	Operational Limit	Cr captures more neutrons than Zr and its transmuted isotopes are high energy Beta emitters; CRUD deposition and adherence will contribute to dose levels; simple analysis on its activation and preliminary data on CRUD should address this data gap.

Relevant Standards

The following is a summary of relevant standards for metallic coatings collected by UW. New standards may be needed depending on how coating role is defined in operational and safety performance of the fuel.

- Adhesion testing
  - ASTM B571-18: Standard practice for qualitative adhesion testing of metallic coatings
    - Includes the following tests: bend, burnish, chisel/knife, draw, file, grind and saw, heat/quench, impact, peel, push, scribe/grid
    - Several of these tests are limited to specific types of coatings, thickness ranges, ductilities, or compositions of the substrate
    - These tests could also be performed after irradiation exposure or burnup limit
  - ASTM C633-13: Standard test method for adhesion or cohesion strength of thermal spray coatings
    - Determines degree of adhesion/bonding strength of a coating to a substrate or cohesion strength of coating in a tension normal to the surface
    - The test consists of coating one face of a substrate fixture, bonding this coating to the face of a loading fixture, and subjecting this assembly of coating and fixtures to a tensile load normal to the plane of the coating
    - This test is usually performed at ambient temperature; higher temperature testing is restricted by the need for a suitable bonding agent
    - A tensile load is applied to the test specimen at a constant rate of cross-head travel between 0.030in/min and 0.050 in/min until rupture occurs; record the maximum load applied
    - Calculate the degree of adhesion/cohesion strength as follows:
      - Adhesion or cohesion strength = maximum load/(cross-sectional area)
- Thermal Diffusivity
  - ASTM E1461-13: Standard test method for thermal diffusivity by the flash method
    - Determines the thermal diffusivity of primarily homogeneous isotropic solid materials, with values ranging from 0.1 to 1000 $(mm)^2s^{-1}$ measureable from about 75 to 2800 K
    - A small, thin disc specimen is subjected to a high-intensity short duration of radiant energy pulse

        - The energy of the pulse is absorbed on the front surface of the specimen and the resulting rear face temperature rise (thermal curve) is recorded
        - The thermal diffusivity value is calculated from the specimen thickness and the time required for the rear face temperature rise to reach a percentage of its maximum value
        - **Also see E2585 for detailed information regarding use of the flash method
- Corrosion
    - ASTM G2/G2M-06: Standard test method for corrosion testing of products of Zr, Hf, and their alloys in water at 360 °C or in steam at 400 °C
        - Specimens are exposed to high-pressure water or steam at elevated temperatures for 72 or 336 hrs
        - The corrosion is normally measured by the gain in mass of the specimens and by the appearance of the oxide film on the specimen surfaces.
        - When so specified, appearance of the specimen shall be the sole criterion for acceptance
- Thermal Cycling
    - ISO 14188:2012: Test methods for measuring thermal cycle resistance and thermal shock resistance for thermal barrier coatings
        - Measures thermal cycle resistance by using steady cyclical heating and cooling procedures
        - Measures thermal shock resistance using a heating and quenching technique
        - Evaluates durability of thermal barrier coatings to thermal strain
- Thermal Shock Resistance
    - ASTM C1525-18: Standard test method for determination of thermal shock resistance for advanced ceramics by water quenching
        - Rapid quenching of test specimen at elevated temperature in water bath at room temperature
        - Thermal shock assessed by measuring reduction in flexural strength
        - Does not determine thermal stresses or thermal expansion mismatch

Other tests

- Ring Compression Test
    - A method for determining a material’s flow stress and the friction factor at the die/specimen interfaces during the compression of ring specimens between flat dies
        - Can qualitatively observe if coating spalls after compression
        - Can qualitatively assess if ductility is improved with the addition of a coating
- Pressurized Burst Test
    - Coated cladding concepts can be tested in a high temperature furnace with elevated internal pressure until cladding bursts
    - Tests can be performed pre- and post-irradiation
- Fretting Wear

- o Fretting wear tests assess the wear resistance of the coated cladding as compared to conventional Zr-alloy cladding
  - o Tests could be standard pin-on-disk wear testing, or a more advanced fretting wear mechanism can be built
  - o Tests can be performed in ambient air environments or in an aqueous or corrosive environment
  - o Tests can be performed pre- and post-irradiation
- Measurement of porosity and adhesion via microscopy techniques
- Testing of mechanical properties after moderate and high temperature steam tests

Test Facilities

It is expected that traditional out-of-pile capability available to the vendors combined with the ATR PWR loops and TREAT facility will be sufficient to address majority of concerns at an accelerated timeline. For post-testing of the irradiated fuel rods, ORNL is also equipped with post irradiation LOCA and mechanical testing capability to address potential postulated concerns regarding coating in areas of local ductility and bursting. A snapshot of Framatome irradiation program is shown below as a reference. If severe accident testing is pursued then FZK facilities in Germany can be leveraged.

EATF Cr_2O_3-enhanced Fuel / Cr-Coated Clad Irradiation Program

Reactor	Sample Type	PIE	Timeline
OSIRIS – CEA*	Cr-coated tubes and flat specimens	Coating performance, adherence	2015-2018
HALDEN – Norway*	Cr-coated rodlets with UO_2 pellets	Coating performance, pellet-clad interaction	2017-2021
IMAGO - Commercial Reactor	Cr-coated tubes, flat specimens, strained samples	Corrosion kinetics, coating performance, mechanical properties..	2016-2022
ATR - INL	Cr-coated rodlets with Cr_2O_3-enhanced pellets	Microstructure, oxidation, hydrogen pickup, coating performance	2018-2022
ORNL	Cr-coated cladding	Mechanical properties	2018-2020
LaSalle	Lead Fuel Assemblies Cr_2O_3-enhanced pellets	Pool side examination Hot Cell	2018 2019-2020
Vogtle - LTAs	Cr-coated rodlets with Cr_2O_3-enhanced pellets	Coating performance, adherence	2019-2024

*French R&D Cooperation Program

Framatome EATF Program – K. Nimishakavi – Feb 2018

Property of Framatome - © Framatome All rights reserved

p.8 framatome

Beyond Current Fuel Licensed Limits

Two potential economic saving strategies commonly pursued under the ATF programs by Utilities are briefly discussed. While the nature of above recommended testing are confirmatory, these potential areas will likely require a large database to show reproducibility and performance of the fuel during a wide range of AOOs and accidents. It should be noted that there are many other strategies that could be viable under this section that are not discussed such as change in critical-heat flux criteria to a cladding time-at-temperature and stress criteria due to better protection of the cladding and Alternate Source Term (AST) regulatory guide as ATF may delay or reduce the type of radionuclide release that impacts plant PRAs and emergency planning zones.

Increase in Zircaloy PCT limit

Given the slower oxidation kinetics of the Cr-coating, the limitation imposed by PCT limit of Zircaloy (2200 ^{o}F) on current tech specs on many plant components such as start time for diesel generators could be relaxed. However, such increase will require more extensive testing than listed above:

1. PIE of "limiting" fuel rods at high burnup (>60 MWd/kgU). The limiting rod could be defined by rod undergoing maximum wear or experiencing highest localized stresses. The latter requires separate effect testing for precise prediction of local stresses in coating to that could give insight in its structural integrity. The PIE must include LOCA testing to ensure the proposed new PCT limit does not result in severe degradation of the cladding.
2. Control rods, grids and core upper structure integrity needs to be revisited as the new proposed PCT will expose these structures to higher temperatures for longer time period.

It is likely that prototypic testing will be required to demonstrate the burden of proof in ability of coated cladding to maintain a higher PCT limit. This will limit the reliance on data generated from test reactors and will take 8-10 years after the initial licensing to realize such benefits while the underlying safety benefits would exists.

Increase in Fuel Burnup Limit

The current burnup limit of fuel rods (~62 MWd/kgU) from cladding point-of-view is primary limited by the cladding oxidation and hydrogen pickup. The coating should improve the oxidation while the hydrogen pickup remains uncertain. Although, for the most efficient core design, many plants in the US (particularly PWRs) are also limited by UO_2 5% enrichment limit. Nevertheless the coating could potentially allow higher burnups and reduce the overall fuel cycle cost. If such strategy is pursued then more extensive testing is required beyond what is recommended above:

1. Thermal-mechanical properties of UO_2 for the proposed burnup limit will need to be obtained with particular attention to high burnup fuel fragmentation.
2. PIE of rods at the new proposed limit for burnup. Particular attention needs to be made on coating adherence and ability to examine coating thickness during the PIE at high burnup to measure its ductility, burst strength, oxidation and hydrogen pickup.
3. Rod ejection testing to ensure UO_2 integrity at higher local burnup.
4. Assessment of role of high burnup structure on fuel post-burst behavior and PCMI in terms of its post-burst wash-out, gas release and overall plant dose profile.
5. Severe accident consideration in terms of overall plant dose release at the proposed higher burnup limit needs to be made.
6. Back-end fuel cycle implication in terms of dose release in pools and eventual disposal (dry cask).